ENVIRON

MEMORANDUM

To: Gerald Dilley, Regional Air Quality Council (RAQC)

From: Ralph Morris and Gerard Mansell

Date: October 12, 2003

Subject: Preliminary CAMx Base Case ozone modeling for the June-July 2002 Denver ozone episode

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INTRODUCTION

The Denver metropolitan area has volunteered to participate in the U.S. Environmental Protection Agency's (EPA) 8-hour ozone Early Action Compact (EAC). Under the 8-hour ozone EAC, the local area volunteers to commit to a program of attainment of the 8-hour ozone by the year 2007. In return EPA will defer designation of the area of nonattainment until after 2007. There are several milestones that must be met in order to satisfy the EAC requirements. One of which is to perform photochemical modeling that can be used to evaluate alternative 8-hour ozone control strategies and demonstrate attainment of the 8-hour ozone standard in 2007.

The Denver Regional Air Quality Council (RAQC) is taking the lead in the Denver 8-hour EAC process. A team consisting of ENVIRON International Corporation and Alpine Geophysics, LLC (ENVIRON/Alpine) has been selected to perform the photochemical modeling for the Denver EAC. Activities of the ENVIRON/Alpine team to date include:

- Development of a Modeling Protocol dated May 21, 2003 that describes the models, episodes and procedures for modeling ozone in the Denver area:
  - The MM5, EPS2x and CAMx models were selected for, respectively, meteorological, emissions and photochemical modeling.
  - The June 7 through July 22, 2002 modeling period was selected that has embedded in it are three 8-hour ozone exceed episodes for Denver:
    - June 8-11, 2002
    - June 25 – July 1, 2002
    - July 18-21, 2002
  - A 36/12 km regional grid covering the southwestern US (from Baja, Mexico in the southwest to southwestern Iowa in the northeast and from Houston, Texas in the southeast to southern Oregon in the northwest) are being used for the entire June 7 through July 22, 2002 period.
  - A 4km grid covering Colorado and a 1.33 km grid covering the Denver area is being used for the three Denver ozone episodes.

- Meteorological modeling was performed using the MM5 model that is documented in a July 1, 2003 report.

- Emissions modeling for the 2002 Base Case and 2007 Future Year was performed using the EPS2x model and data from the Colorado DPHE for Colorado and the NEI99 v2 inventory for outside of Colorado:
  - Link based Vehicle Miles Traveled (VMT) data were obtained from a traffic demand model (TDM) and used along with the MOBILE6 model to generate on-road mobile source emissions for the Denver area.
  - Additional information on emissions from oil and gas activities was obtained from COGA.
  - Biogenic emissions were generated using the GLOBEIS model.
  - The 2002 emissions are documented in a report dated September 19, 2003 and an addendum report dated September 29, 2003.
  - The 2007 emissions were documented in a report dated October 2, 2003.

- The first CAMx base case simulation was completed on September 29, 2003.

PRELIMINARY BASE CASE SIMULATION AND MODEL PERFORMANCE EVALUATION

To date, 10 CAMx sensitivity simulations have been perform using the June/July 2002 modeling database. These simulations are as follows:

Run 1: Preliminary Base Case for the June 7 through July 22, 2002 period on the 36/12 km regional grid.
Run 2: Preliminary Base Case simulation for the June 25 – July 1, 2002 episode on a 36/12/4 km grid.
Run 2a: Preliminary Base Case simulation for the July 18-21, 2002 episode on a 36/12/4 km grid.
Run 3: Preliminary Base Case simulation for the June 25 – July 1, 2002 episode on a 36/12/4/1.33 km grid.
Run 3a: Preliminary Base Case simulation for the July 18-21, 2002 episode on a 36/12/4 km grid.
Run 4: Same as 36/12 km Run 1 only limit mixing heights to 2,000 m AGL and add Kvpatch minimum to layer 1.
Run 5: Same as 36/12 km Run 1 only with reprocessed emissions to include VOC speciation profiles provided by COGA for Flash VOC emissions in Weld County and to correct some Colorado mobile source emissions where 2007 emissions were mistakenly provided in the 2002 inventory.
Run 5a: Run 5 only on a 36/12/4 km grid and for the June 25 – July 1, 2002 episode.
Run 5b: Run 5 only on a 36/12/4 km grid and for the July 18-21, 2002 episode.
Run 6: Restructured vertical layer configuration. Run aborted after little improvement in model performance seen in first part of episode.

The CAMx model using a 36/12 km grid requires 1.5 to 3 CPU hours per simulation day. Thus, the 46 day June 7 through July 22, 2002 episode requires a little over 3 CPU days to complete. Using the 36/12/4 km grid, the CAMx model requires approximately 11 CPU hours per simulation day to run. Thus, the 7 day June 25 through July 1, 2002 and 4 day July 18-21, 2002 episodes require approximately 3.2 and 1.9 CPU days to run, respectively. On the 36/12/4/1.33 km grid, the model requires approximately 16 CPU hours per simulation day so that the two episodes required approximately 4.9 and 2.7 CPU days to complete. Thus in total, running the entire June 7 through July 22, 2002 episode with the highest resolution grid during the two 8-hour ozone episodes (i.e., 36/12/4/1.33 km) requires approximately 11 CPU days to complete with an additional 5 CPU days needed if the 36/12/4 km grid is also desired for the two episode periods.

When the model-ready emission inventories were ready around the end of September, the CAMx base case simulation was initiated that include the first 5 runs running at all 3 grid resolutions in the Denver metropolitan area. In hindsight, a more staged approach for running the model at the different resolutions with intermediate analysis may have been a more optimal approach, however the aggressive time schedule of the Denver 8-hour ozone EAC did not accommodate a more thoughtful and methodical approach. Thus considerable effort and computer time (~16 CPU days) was expended running the model at the three grid resolutions to meet the EAC schedule.

EPA Model Performance Evaluation Guidelines and Goals

EPA has published draft 8-hour ozone modeling guidelines (EPA, 1999) that are used initially as a basis, in part, for judging the adequacy of the Denver base case simulation. As discussed in the Denver 8-hour ozone EAC Modeling Protocol (Tesche et al., 2003), model performance evaluation should be considered as a series of tests that become more stringent as one moves through the model performance process. We are using the EPA draft 8-hour modeling guidelines as an initial test of model performance. These tests focus primarily on ozone model performance. After applying the EPA's performance tests to the model, the model performance moves on toward more stringent tests that can include comparisons of ozone precursors with available data, comparisons of VOC speciation, ozone indicator comparisons as available, and further diagnostic tests. If the model does not achieve a level of performance in the initial tests, then corrective action and further diagnostic tests are usually performed to identify the problem(s) and take corrective action. Such corrective action can range from simple adjustments, like accounted for drought stress in biogenic emissions and dry deposition or eliminating wet scavenging due to uncertain convective cloud systems, to more intensive tests that may include rerunning the meteorological model or identifying and quantifying missing emissions from the inventory.

There are two main components in EPA's draft 8-hour ozone guidance operational ozone model performance that we are using as an initial test of model performance: (1) Big Picture Assessment Using Graphics; and (2) Ozone Metrics.

Big Picture Assessment Using Graphics

EPA's draft 8-hour ozone guidance lists four graphic displays that are used to obtain a big picture of model performance:

- Tile plots of observations and predictions: These are used to understand the spatial differences and displacements of the predicted and observed ozone concentrations and to compliment the ozone metrics. For example, an ozone plume that is displaced a little from the ozone monitor may produce very poor ozone metrics but may still be a reliable tool for control strategy evaluation if the correct sources and processes are being simulated to produce accurate peak ozone that is just displaced from the monitor. These plots can be used to assess model performance upwind and downwind of the Denver urban area to assist in interpreting performance issues die to transport versus local photochemical production.

- Tile plots of differences in observations and predictions: Combined with the tile plots of absolute predicted and observed concentrations above this plot may provide some insight into performance under low and high ozone concentrations. Given the limited ozone network in the Denver area, the same information from this plot can be obtained by the absolute concentrations plots.

- Scatter plots and quantile-quantile (Q-Q) plots: Scatter plots provide a measure of how well the model is replicating the observed ozone concentrations at or in the vicinity of the monitor. Q-Q plots provide a measure of how well the model is reproducing the frequency distribution of the observed ozone concentrations.

- Time series plots: Time series plots of predicted and observed hourly ozone concentrations provide a stringent test of how well the model replicates the observed hourly ozone at the same time and location as the observed value. Problems with temporal timing in the model are readily apparent in a time series plot.

Ozone Metrics

EPA's draft 8-hour ozone guidance identifies several ozone metrics to be applied to the model along with performance goals that should be met. Table 1 below lists EPA's performance test, performance goal and a comment on how the model will be tested using this test in the Denver 8-hour ozone EAC modeling.

Table 1. EPA's draft 8-hour ozone modeling guidance ozone performance tests and goals and how they are applied.

Test(s)	Goals/Objectives	Comment
"bias pred/obs mean 8-hr (& 1-hr) daily maxima near each monitor"[1]	"~20% most monitors (8-hr comparisons only)"[1]	EPA's draft modeling guidance does not define "near each monitor". After discussing this issue with EPA "near" was defined to mean the same block of grid cells near the monitor used in EPA's attachment test (e.g., 7 x 7 for 5 km grid). There are three ways we defined "near" for this metric: (1) Select the maximum predicted daily maximum 8-hr ozone concentrations "near" the monitor; (2) Select the predicted values closest in value to the observed value "near" the monitor; and (3) Select the predicted value at the monitor.
"fraction bias pred/obs mean 8-hr (& 1-hr) daily maxima near each monitor"[1]	"~20% most monitors (8-hr comparisons only)"[1]	Define "near" the three ways described above.
"correlation coefficients, all data, temporally paired means, spatially paired means"[1]	"moderate to large positive correlations"[1]	Apply to three data sets described above.
"bias (8-hr daily max and 1-hr obs/pred), all monitors"[1]	"~5-15%"[1]	
"gross error (8-hr daily max and 1-hr obs/pred), all monitors"[1]	"~30-35%"[1]	
Partition data base into upwind, center city and downwind sites and repeat analysis		Get better ideas of level of model agreement based on upwind/downwind stratification and whether there is any obvious pattern of the model performance.
"Scatter plots & Q-Q plots of 8-he and 1-hr metrics"		Applied to three sets of databases listed above.

1 "Draft Guidance on the use of Models and other Analysis in Attainment Demonstrations of the 8-Hour Ozone NAAQS" (EPA, 1999)

Additional Measures of Model Performance

Once the model performance tests listed above are applied, additional performance tests may be applied depending on schedule and resource constraints. The application of these performance tests have not yet been undertaken so are not discussed in this document but they include:.

- Comparisons of secondary species (e.g., NO2, NOy, NOx, NOz).
- Comparisons of ozone precursors (NOx , VOC, CO and VOC speciation).
- Comparisons of ratios of co-varying species (VOC or VOC/CO, VOC species/CO, VOC/NOx, etc.).
- Spatially averaged predictions of the above or of primary species.
- Comparison of modeling results with Observation Based Models (OMB) (e.g., CMB, multivariate models, extent parameter, etc.).
- Comparison of weekday versus weekend day effects.
- Ratios of key indicator species (e.g., O3/Noy, O3/Noz, O3/HNO3, H2O2/HNO3).
- Retrospective analysis.

Preliminary Model Performance Evaluation for Initial Configuration

The initial configuration of the CAMx model included running at the three grid resolutions (36/12, 36/12/4 and 36/12/4/1.33 km) using the first set of processed emissions that did not include the COGA VOC speciation data for the Weld County Flash emissions that were received to late to include in the initial emissions modeling and included 2007 Vehicle Miles Traveled (VMT) data for some Colorado Counties that were mistakenly labeled as 2002.

Below we present the performance evaluation of the initial CAMx base case simulation using EPA's modeling guidance performance tests.

Tile Plots of Observations and Predictions

Attachment A displays spatial maps of predicted 8-hour ozone concentrations on the 1.33 km grid domain for the two episodes: June 25 through July 1, 2002 and July 18-21, 2002.

June 25, 2002: On June 25, 2002 the peak observed 8-hour ozone concentration was 81 ppb at the Rocky Flats monitor. Adjacent to this monitor was an 8-hour ozone observed value of only 68 ppb at Boulder on this day. The model estimates values of 55-65 ppb at these two locations.

North of the Rocky Flats monitor on the border of Boulder and Larimer Counties the model is estimating daily maximum 8-hour concentrations of 75-85 ppb. In the immediate Denver metropolitan area the peak observed 8-hour ozone concentrations is 75 ppb at the NREL monitor. Although the model estimates 8-hour ozone values in the 55-65 ppb at the NREL monitor, a few grid cells to the southwest of the NREL monitor the model estimate values of 65-85 ppb. The other Denver monitors have lower observed 8-hour ozone concentrations (58-68 ppb) that agree somewhat with the predictions (45-75 ppb). However, the model appears to estimate a higher level of suppression of ozone in downtown Denver (68 ppb observed vs. 45-55 ppb predicted) that is likely due to NOx suppression of ozone formation that could be due to insufficient mixing, understated VOC emissions, overstated NOx emissions, understated photolysis rates (e.g., overstated clouds), or other factors.

<u>June 26, 2002</u>: The peak observed 8-hour ozone concentrations in the 1.33 km domain on June 26, 2002 was 81 ppb in Weld County where 45-55 ppb estimated values occurred. The maximum observed 8-hour ozone concentrations in the Denver area was 79 ppb south of Denver at the Chatfield monitor. At this location the model estimates values in the 55-65 ppb. Immediately south of the Chatfield monitor the model estimated values in the 75-85 ppb range occur. Again, the model is overstating the effects of the local suppression of ozone due to NOx emissions in the downtown Denver area that may be due, in part, to the reasons given for the previous day.

<u>June 27, 2002</u>: On June 27, 2002, the spatial displacement of the estimated elevated 8-hour ozone concentrations from the Denver area is not as great as the previous days and consequently better model performance is estimated. The maximum observed 8-hour ozone concentrations in the Denver area (79 ppb at Chatfield) is estimated reasonable well by the model (65-75 ppb) and the high observed value in Boulder (74 ppb) is also reproduced fairly well (~75 ppb), although the lower observed value at Rocky Flats (52 ppb) adjacent to the Boulder monitor is overestimated. Clearly, subgrid-scale processes are affecting the Rocky Flats monitor on this day that can not be reproduced by the model. The observed 8-hour ozone concentrations in the Denver area (62-76 ppb) are reproduced fairly well by the model on this day (55-80 ppb). The overstatement of the local suppression of ozone in the downtown Denver area is not as pronounced on this day as the previous two days.

<u>June 28, 2002</u>: A peak observed 8-hour ozone concentration of 83 ppb occurred at the Chatfield monitor south of Denver on this day. The model also estimates elevated ozone concentrations south of Denver with a value of ~75 ppb at the Chatfield monitor and a peak estimated value of ~85 ppb to the immediate southeast of the Chatfield monitor. The ozone suppression area within the downtown Denver areas again appears to be overstated by the model, which likely accounts for the spatial displacement of the estimated peak occurring further downwind than observed.

<u>June 29, 2002</u>:

<u>June 30, 2002</u>: On June 30, 2002 the model estimates a cloud of elevated (75-85 ppb) 8-hour ozone concentrations that occurs with a southeast to northwest orientation just west of Denver. The observations support the occurrence of such an elevated cloud with observed values of 76,

70, 81, 89 and 81 ppb oriented along the same southeast to northwest orientation. However, the estimated cloud occurs a couple grid cells further west than observed. Thus at the location of the observed peak (89 ppb at Rocky Flats) the model estimates values in the 65-75 ppb range. However, the model exhibits good agreement with the observed values at the Chatfield (78 ppb) and NREL (81 ppb) monitors. The local ozone suppression in the downtown Denver area estimated by the model (55-65 ppb) appears to be overstated based on the observed values (68-72 ppb).

July 18, 2002: On July 18, 2002 the model estimates elevated 8-hour ozone concentrations of 75-85 ppb that occur southwest of Denver. The observed maximum 8-hour ozone values, however, occur immediately west of Denver at the NREL monitor (82 ppb) and to the northwest of Denver at Rocky Flats (78 ppb). The local ozone suppression in the downtown Denver area is overstated by the model (35-55 ppb) compared to the observations (64-70 ppb).

July 19, 2002: On July 19, 2002 the model again estimates that the estimated elevated ozone cloud occurs displaced from the monitoring network to the southwest. The elevated observed values to the northwest of the city at Rocky Flats (93 ppb) and Boulder (87 ppb) are underestimated by the model (55-65 ppb). As are the observed values at the NREL monitor (92 ppb observed vs. 55-65 ppb estimated) and Chatfield (89 ppb observed 75 ppb estimated) monitors. The ozone suppression in the Denver areas is greatly overstated on this day with estimated values of 35-55 ppb occurring where an 84 ppb is observed.

July 20, 2002: The model greatly underestimated the observed 8-hour ozone concentrations on this day. A peak value of only 75 ppb is estimated to occur adjacent to the 83 ppb observed value at Chatfield. However, at the NREL monitor where a 92 ppb 8-hour ozone value is observed the estimated values is only 55-65 ppb are occurring. Again, this is partly due to overstating the suppression of ozone in the Denver areas with estimated values of 35-65 ppb occurring where an 84 ppb is observed.

July 21, 2002: Slightly better model performance is seen on July 21 compared to the previous days with an elevated cloud of 8-hour ozone concentrations of 65-75 ppb estimated immediately southwest of Denver where observed values of 81, 66 and 79 ppb occur. Ozone appears to be underestimated by 5-15 ppb across the network on this day.

An analysis of the comparisons of the predicted and observed spatial distribution of 8-hour ozone concentrations reveals several common themes among the model performance for the episode days.

- The elevated 8-hour ozone plumes are estimated to be of lower magnitude and to occur further displaced from Denver than the observed values.

- The suppression of ozone concentrations in the downtown Denver area is overestimated on almost all episode days. The reasons for this could be multifold:
  - Understatement of local mixing by the MM5 model (e.g., no urban heat island effects) resulting in overstated surface layer NOx and overstated NOx

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suppression.

- Understated VOC emissions inventory due to missing or poorly quantified emissions.
- Overstated NOx emissions.
- Understated ozone and VOC transport into Denver.
- Excessive or incorrectly placed convective activity that results in limited mixing, reduced solar intensity and/or wet scavenging of ozone and precursors.

- There appears to be some spatial misalignment on some days, which is corroborated by the MM5 model evaluation whose wind direction bias on the 1.33 km grid for the June (37 degrees) and July (43 degrees) exceeded the target benchmark values (< 30 degrees).

- During portions of the episodes, the MM5 estimates large amounts of convective activity that reduces mixing and affects transport and diffusion as well as chemistry and scavenging. Although observations generally support the occurrence of some convective activity, it is interesting to note that the model estimates worse model performance during periods of enhanced MM5 estimated convective activity (e.g., beginning of June episode) versus periods of less estimated convective activity (e.g., end of June episode).

- It appears that both ozone transport (regional ozone) as well as ozone produced by local photochemistry is understated by the model on most days.

<u>Scatter Plots, Q-Q Plots and Ozone Metrics</u>

As noted previously, draft EPA guidelines recommends comparison observed daily maximum 8-hour ozone concentrations with predicted values "near" the monitor. After discussing this issue with EPA, "near" the monitor was defined using the same procedures as stated in the 8-hour ozone guidance attainment test; which is a block of grid cells within 15 km of the monitor. Using this definition of "near" and the three procedures for selecting the estimated 8-hour ozone concentrations near the monitor (maximum, best fit and at the monitor) Figures 1 through 3 display the scatter and Q-Q plot results for predicted and observed daily maximum 8-hour ozone concentrations for the 13 monitors in the Denver area and vicinity and the June 2002 Run 2 4-km simulation.

<u>Maximum Estimated 8-Hour Ozone Concentrations Near the Monitor</u>: Figure 1 displays a scatter plot and Q-Q plot comparison using the observed daily maximum ozone concentrations at each monitor during the June 2002 episode and the maximum estimated value "near" the monitor. The EPA performance goal for this metric is that most modeled estimates should be within ∀20% of the observed value. Of the 89 predicted and observed daily maximum 8-hour ozone peaks, 7 pairs exceed the <∀20% EPA performance goal. As shown in Figure 1, most of these values are very close to the goal, some as close as –20.1%. In any event, over 90% of the modeled maximum daily maximum 8-hour ozone concentrations near the monitor are within 20% of the observed value. The r^2 correlation coefficient for these comparisons is 0.31, which provides an r value of around 0.56. The Q-Q plot of 5 percentile quantiles are given by the open

circles in Figure 1 display a general modeled underestimation tendency of the observed 8-hour ozone frequency distribution at the high end of between 0 and –20%.

Best Fit Estimated 8-Hour Ozone Concentrations Near the Monitor: Figure 2 displays the predicted and observed daily maximum 8-hour ozone concentrations for the June 2002 episode and Run 2 (4 km simulation) using the closest estimated value "near" the ozone monitor. Again the EPA performance goals is that most estimated 8-hour ozone concentrations be within 20% of the observed value and this is achieved at over 90% of the predicted/observed pairs. As for the maximum comparisons, there is an underestimation bias at the high observed end where the Q-Q plots lies between 0 and –20%.

Spatially Paired Estimated 8-Hour Ozone Concentration: Figure 3 displays a comparison of the predicted and observed daily maximum 8-hour ozone concentrations spatially paired at the monitor location for the June 2002 episode and Run 2 (4 km). Note that EPA's within 20% performance goal are for comparisons near the monitor so do not apply to this more stringent test. However, it is useful to examine the spatially (at monitor) and temporally (by day) paired predicted and observed daily maximum 8-hour ozone concentrations to gain insight into the simulation. Not surprising given the discussion of the spatial maps, the model underestimates the observed 8-hour ozone concentrations by approximately 20% across the frequency distribution of the observed values. Attachment B displays scatter plots of spatially paired predicted and observed daily maximum 8-hour ozone concentrations for the June and July 2002 episode periods. As seen in the spatial maps (Attachment A), the model is estimating better spatial alignment with the observed 8-hour ozone concentrations during the June than July 2002 episode. During the June episode, the 1:1 line of perfect agreement bisects the predicted and observed daily maximum 8-hour ozone concentrations scatter plot for each day during the June episode (Attachment B). Whereas, for the July episode, the scatter plot points are almost always on the underprediction side of the 1:1 line (Attachment B).

Time Series Analysis

Figures 4 displays time series of estimated and observed 1-hour ozone concentrations averaged across all monitors within the 1.33 km modeling domain (see Attachment A). These time series confirm that the model is underestimating the afternoon ozone concentrations by a fair margin. As discussed previously, this underprediction is due in part to spatially displacement of the estimated ozone plume away from Denver, the overstatement of the ozone suppression in the Denver metropolitan area, the underestimation of ozone and precursor transport ,and other reasons to be determined.

Effects of VOC Speciation and On-Road Mobile Source Updates

As noted previously, the VOC speciation for Flash emissions from Weld County was provided too late to incorporate into the first Base Case simulations. Also, for some counties in Colorado incorrect VMT data were provided. These updates would be expected to provide little change in the general model performance. However, concerns were raised that these data weren't included so the Weld County VOC speciation data were analyzed and incorporated into the analysis and Run 5 was performed on the 36/12 km grid and the June 7 through July 22, 2002 episode. Additional runs for the June and July 2002 episodes were also initiated on the 36/12/4 k grid, but were unavailable for this document.

Attachment C displays running 8-hour ozone time series of predicted and observed concentrations using 12 km grid estimates for Run 1 and Run 5 (corrected Weld County Flash VOC emissions speciation). These time series show that the model underestimates the very highest observed 8-hour ozone concentrations. They also show that the Flash emissions VOC speciation has no effect on the estimated ozone concentrations at the monitors using the 36/12 km model configuration.

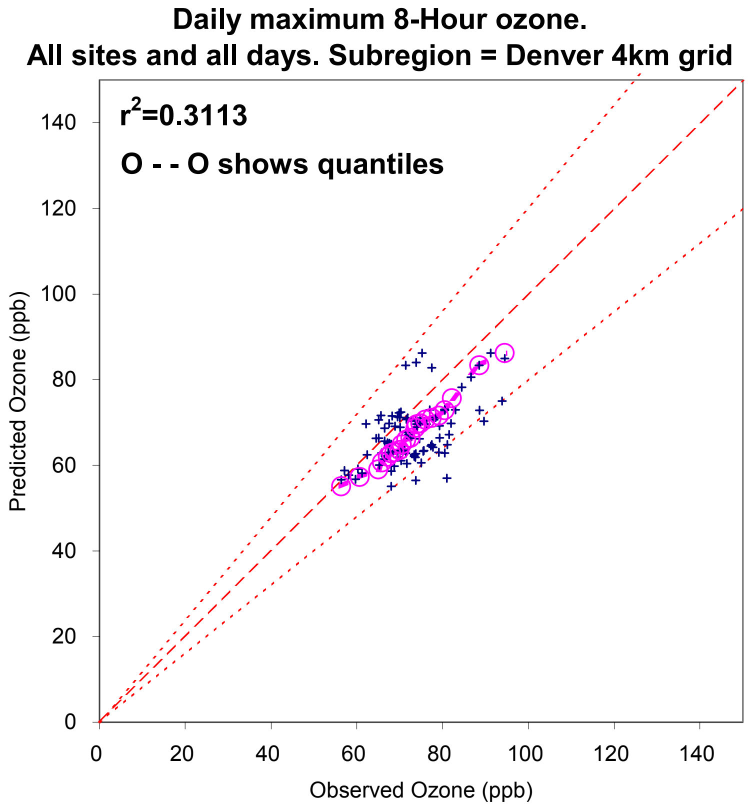


Figure 1. Comparison of predicted and observed daily maximum 8-hour ozone concentrations using the predicted maximum near the monitor for sites in the Denver region and the 4 km Run 2 simulation of the June 2002 episode.

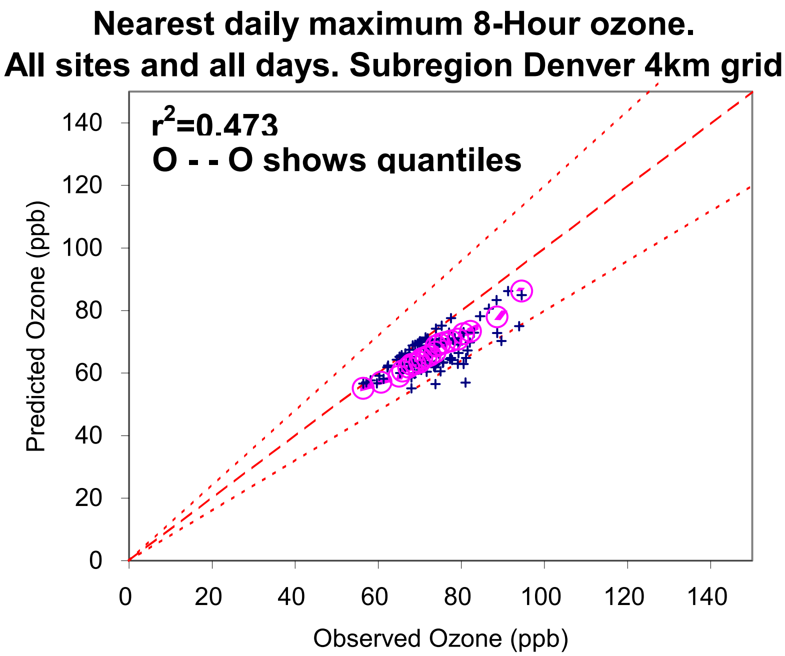


Figure 2. Comparison of predicted and observed daily maximum 8-hour ozone concentrations using the predicted best fit near the monitor for sites in the Denver region and the 4 km Run 2 simulation of the June 2002 episode.

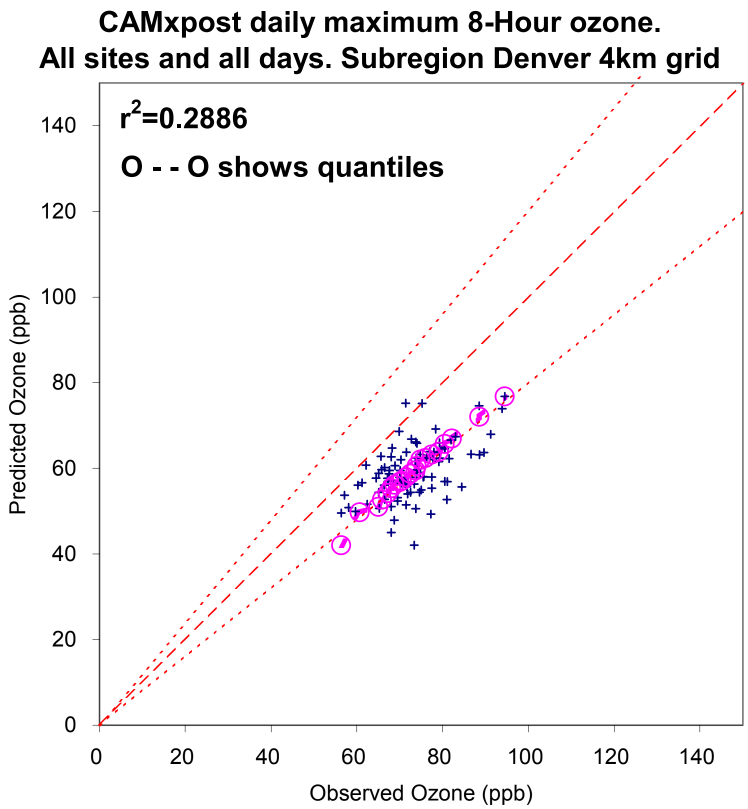


Figure 3. Comparison of predicted and observed daily maximum 8-hour ozone concentrations using the predicted value at the monitor for sites in the Denver region and the 4 km Run 2 simulation of the June 2002 episode.

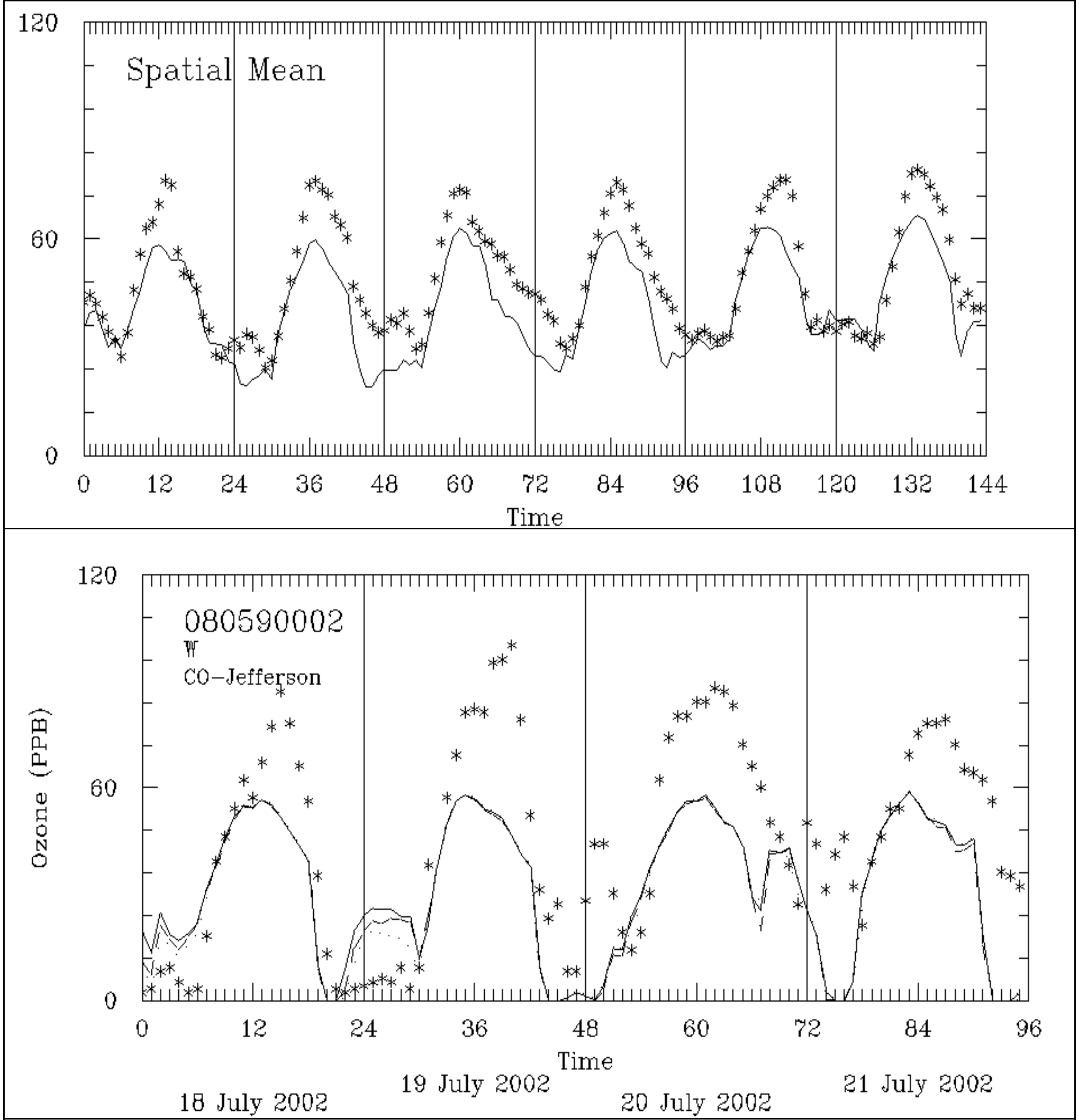


Figure 4. Predicted and observed spatially averaged 1-hour ozone concentrations for the 1.33 km grid and Run 3 June 2002 episode (top) and Run 4 July 2002 episode (bottom)

CONCLUSIONS AND RECOMMENDATIONS

The current Denver 8-hour ozone Base Case simulation for the June/July 2002 episodes achieves EPA's draft 8-hour ozone modeling guidance performance goal of estimating predicted daily maximum 8-hour ozone concentrations near the monitor to within ∀20% of the observed value at most monitors. However, more detailed analysis of model performance reveals several performance issues that should be addressed in order to have a more reliable ozone modeling tool for 8-hour ozone planning. Some of the major performance issues are as follows:

- The model exhibits a spatial displacement of the elevated ozone concentrations further away from the Denver metropolitan area than observed.
- Overstatement of the afternoon ozone suppression in the Denver metropolitan area on most days.
- Underestimation of ozone transport into the Denver metropolitan area.
- Underestimation of the amount of local photochemical production due to local emissions.
- Overstatement or misallocation of local convective activity during some days of the episode.
- Other as yet unidentified performance issues.

Causes for many of these phenomena may include:

- Understated mixing in the Denver area.
- Overstated maximum afternoon mixing heights.
- Understated VOC emissions inventory or understated VOC reactivity (local and/or regional).
- Overstated local NOx emissions.
- Understated ozone and/or VOC boundary conditions (BCs).
- Wind direction and wind speed errors.
- Other causes.

Recommendations

As part of the development of SIP quality photochemical modeling databases it is fairly typical that the first photochemical grid model Base Case simulation uncovers issues in the meteorological and emission fields that should be improved. The rerunning of the meteorological model with alternative Planetary Boundary Layer (PBL) or Land Surface Module (LSM) schemes and/or with different levels of Four Dimensional Data Assimilation (FDDA) to generate more representative meteorological inputs is routinely performed as part of the development of a SIP quality modeling database. The photochemical model is also a good diagnostic tool for identifying uncertainties and/or omissions in the emissions database or inappropriate boundary conditions (BCs). The following are some recommended actions aimed at improving the ozone model performance using technical justifiable approaches.

Meteorology

A series of MM5 sensitivity model simulations should be undertaken aimed at improving the representation of the Front Range meteorological and improving the CAMx model performance in the Denver area and vicinity. However, the study design of the Denver 8-hour EAC developed by the sponsors precludes such actions without modifications to the study's schedule and resources. As currently designed by the Denver EAC sponsors, only ad hoc adjustments to the existing meteorological inputs can be undertaken and the amount of analysis is extremely limited under the current study design.

It is highly recommended that sufficient time and resources are allocated to properly generate the meteorological fields needed to simulate ozone in the Front Range region. However, under the current study design of the EAC sponsors the following ad hoc adjustments to the existing meteorological fields should be examined and if technically justified adopted as a new Base Case configuration:

- Examine the level of mixing within the Denver metropolitan area to account for the effects of the urban heat island, mechanical mixing and understated mixing due to incorrect characterization by MM5.

- Examine the level of mixing outside of the Denver metropolitan area and determine whether it is over or understated and develop correction factors.

- Perform sensitivity tests without wet deposition and/or without clouds attenuation of photolysis rates to determine whether overactive convective activity is contributing to the ozone underestimation.

Emissions

The overstatement of the ozone suppression in the Denver area could likely be due in part to overstated local NOx emissions or understated local and/or regional VOC emissions. The understated ozone transport may be due in part to understated regional VOC and/or NOx emissions.

Recent measurements report that methane, ethane and alkane emissions from oil and gas development activities are understated in the Anadarko Basin that includes Texas, Oklahoma and portions of New Mexico and Colorado (Katzenstein et al., 2003). Although methane has very low reactivity and ethane is classified as non-reactive, they do have some reactivity. In fact, in the CB-IV chemical mechanism, the 2 carbons in ethane are speciated as 0.4 PAR (i.e., 20% of the reactivity of a typical alkane). Given the shear magnitude of these emissions through out the region upwind of Denver, they should be accounted for to develop more precise and reliable ozone control plans.

Thus it is recommended that a review of the emissions inventory to identify and quantify missing emissions, including regional VOC and ethane emissions, be undertaken. Given the time and resource constraints imposed by the EAC sponsors, only cursory analysis can be addressed using sensitivity analysis under the current study plan.

- After improving the meteorology, perform sensitivity analysis that increases local VOC and/or decreases local NOx emissions in the Denver area.

- Develop a "place holder" inventory that adds a regional emissions inventory of alkane emissions in the CO/NM/OK/KS/TX region to account for the undocumented and uncharacterized alkane and ethane emissions as discussed by Katzenstein and co-workers (2003).

Transport

The underestimation of ozone transport may be due in part to understated regional emissions discussed above and/or overstated mixing and/or other possible factors. Along the outer edge of the 36 km modeling domain, fairly clean values of ozone, NOx and VOC of approximately 40 ppb, 1.1 ppb and < 10 ppbC are specified. Note that the article by Katzenstein et al., (2003) suggest these VOC BCs are greatly understated. These values likely understate regional ozone concentrations along portions of the northern and eastern boundaries during the June/July 2002 episode. This suggest the following:

- Perform sensitivity test with increases BCs along portions of the northern and eastern boundaries. Particular focus should be on the VOC and ozone BCs.

- If the above sensitivity test exhibits ozone sensitivity in the Denver area, then more refined BCs should be developed based on available measurements.

Conclusions

Given the time and resource constraints of the current EAC study design imposed by the project sponsors, not all of the activities above can be completed under current time and resource constraints. Thus, it is recommended that two activities be undertaken in parallel:

(1) Continue improving the base case modeling database under the current schedule and resource constraints to achieve a first guess of the level of additional control (if any) needed to achieve attainment in 2007; and

(2) Initiate a longer term analysis designed to refine the first guess control strategy as new and better information and improved databases are developed.

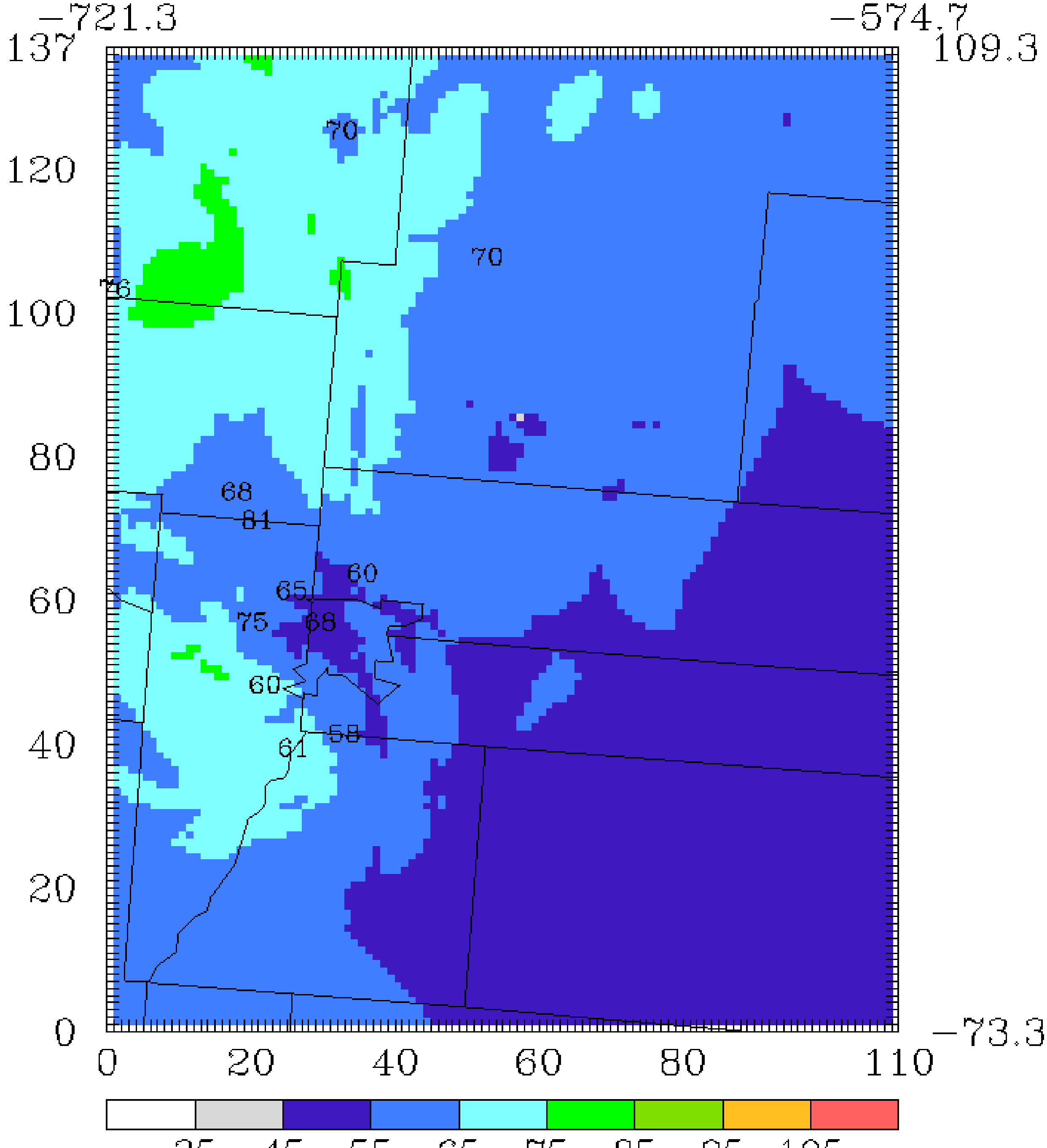
Golden Gate Plaza $ 101 Rowland Way $ Novato, California 94945-5010 USA
Tel: (415) 899-0700 $ Fax: (415) 899-0707

Attachment A

Distribution of predicted and observed daily maximum 8-hour ozone concentrations for the Preliminary Base Case simulation on the 4 km rid and:

Run 2: June 25 through July 1, 2002 episode
Run 2a: July 18-21, 2002 episode

Max value: 7.933E+01 at (10,104)
Min value: 4.494E+01 at (58, 86) non zero cells only
Avg value: 5.933E+01 non zero cells only
Grid Total: 8.650E+05

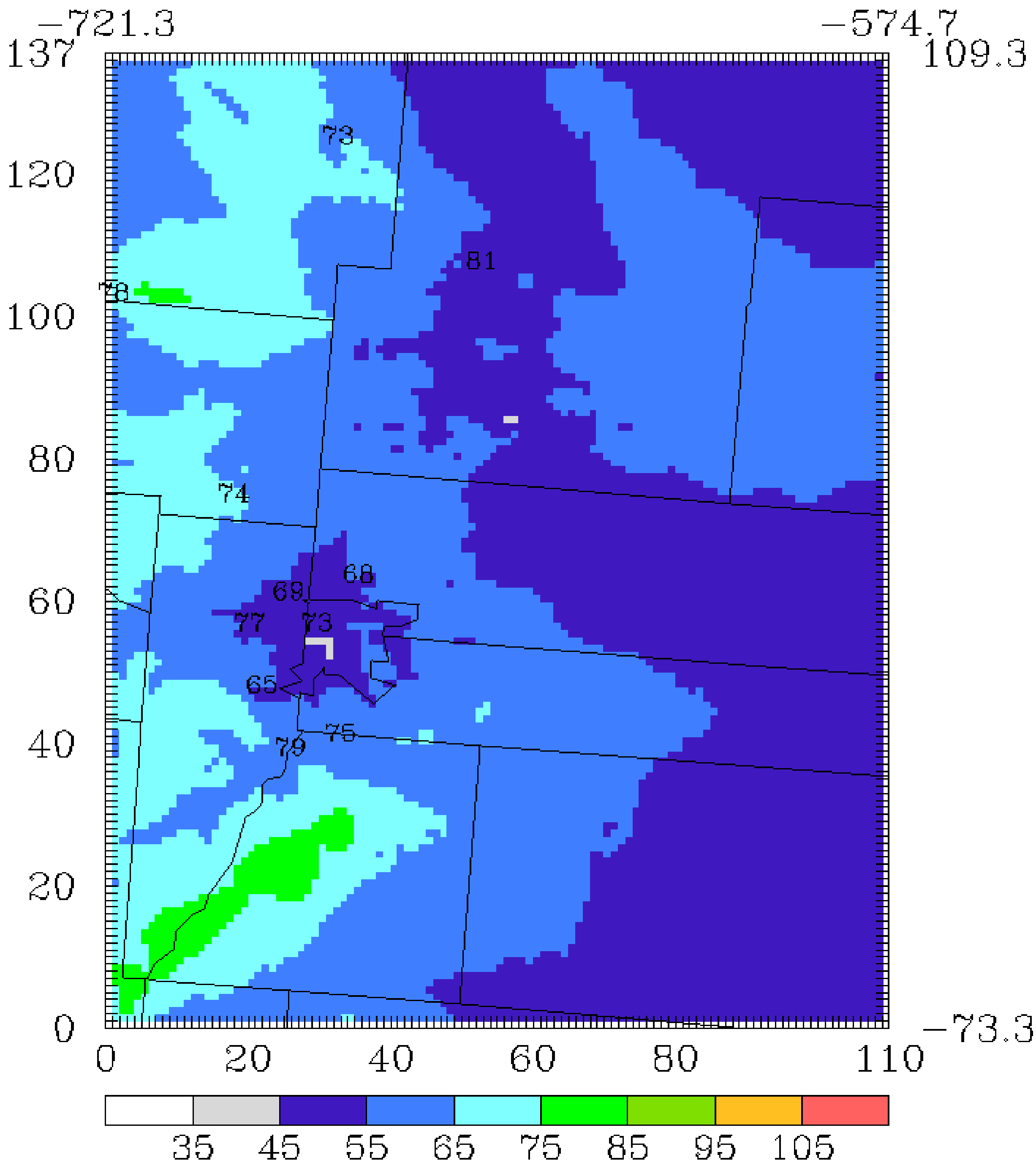


Daily Max. 03 Concentration (ppb)

20020625 : 9999

8 Hour Average

Max value: 8.240E+01 at (24, 23)
Min value: 3.528E+01 at (58, 86) non zero cells only
Avg value: 5.816E+01 non zero cells only
Grid Total: 8.480E+05

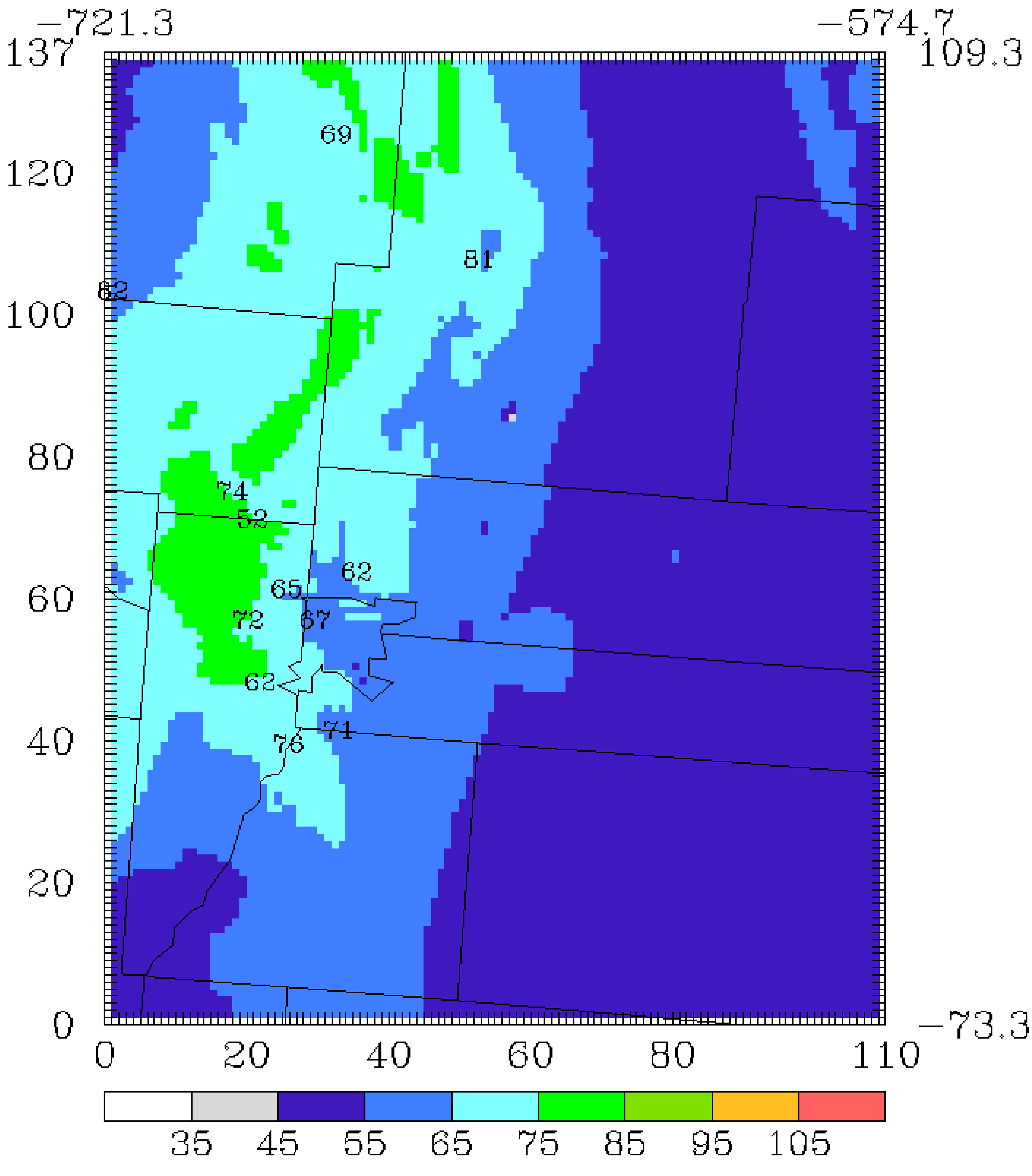


Daily Max. O3 Concentration (ppb)

20020626 : 9999

8 Hour Average

Max value: 8.493E+01 at (16, 64)
Min value: 4.218E+01 at (58, 86) non zero cells only
Avg value: 5.923E+01 non zero cells only
Grid Total: 8.636E+05

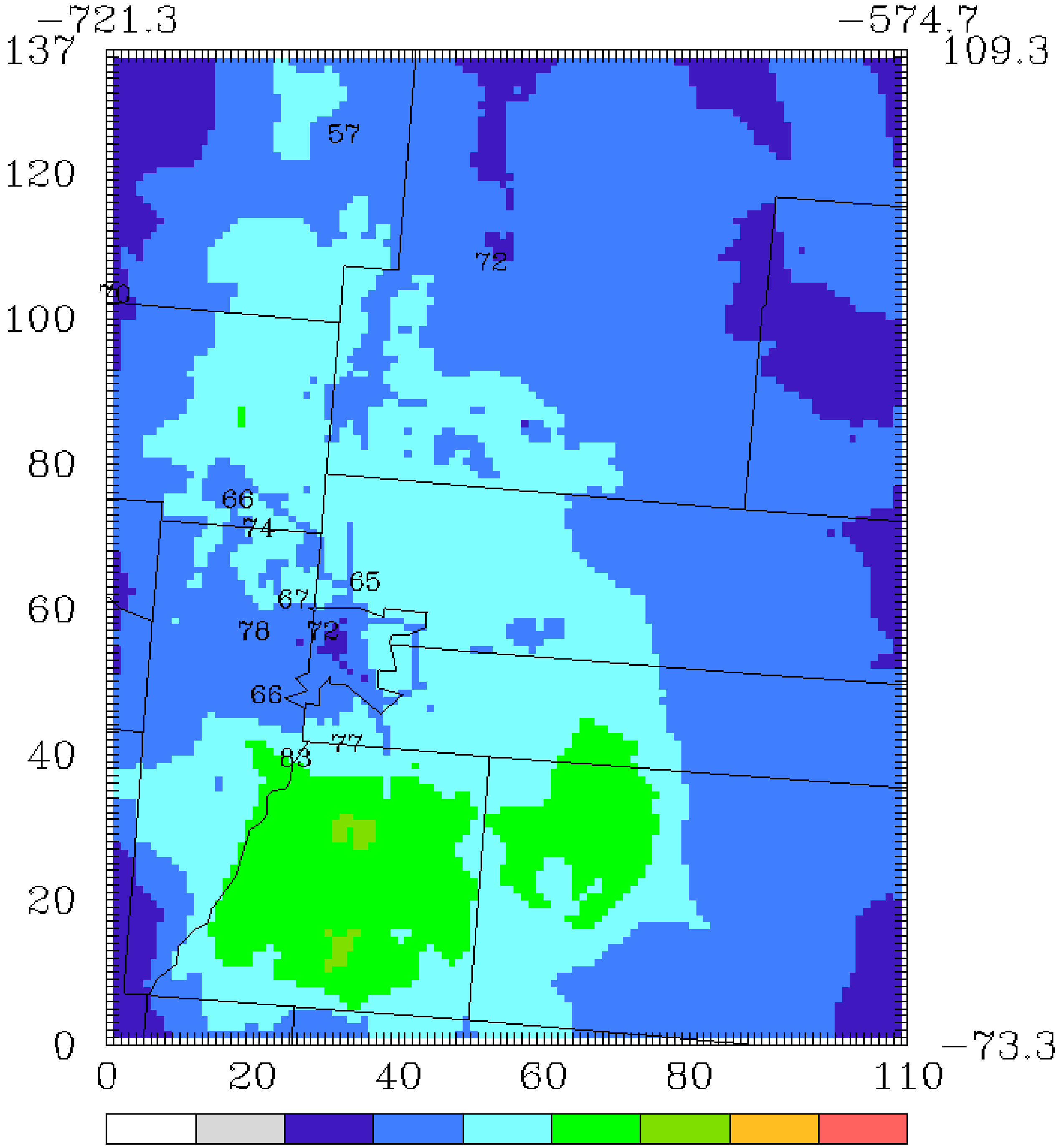


Daily Max. O3 Concentration (ppb)

20020627 : 9999

8 Hour Average

Max value: 8.750E+01 at (32, 13)
Min value: 4.859E+01 at (3,130) non zero cells only
Avg value: 6.341E+01 non zero cells only
Grid Total: 9.245E+05

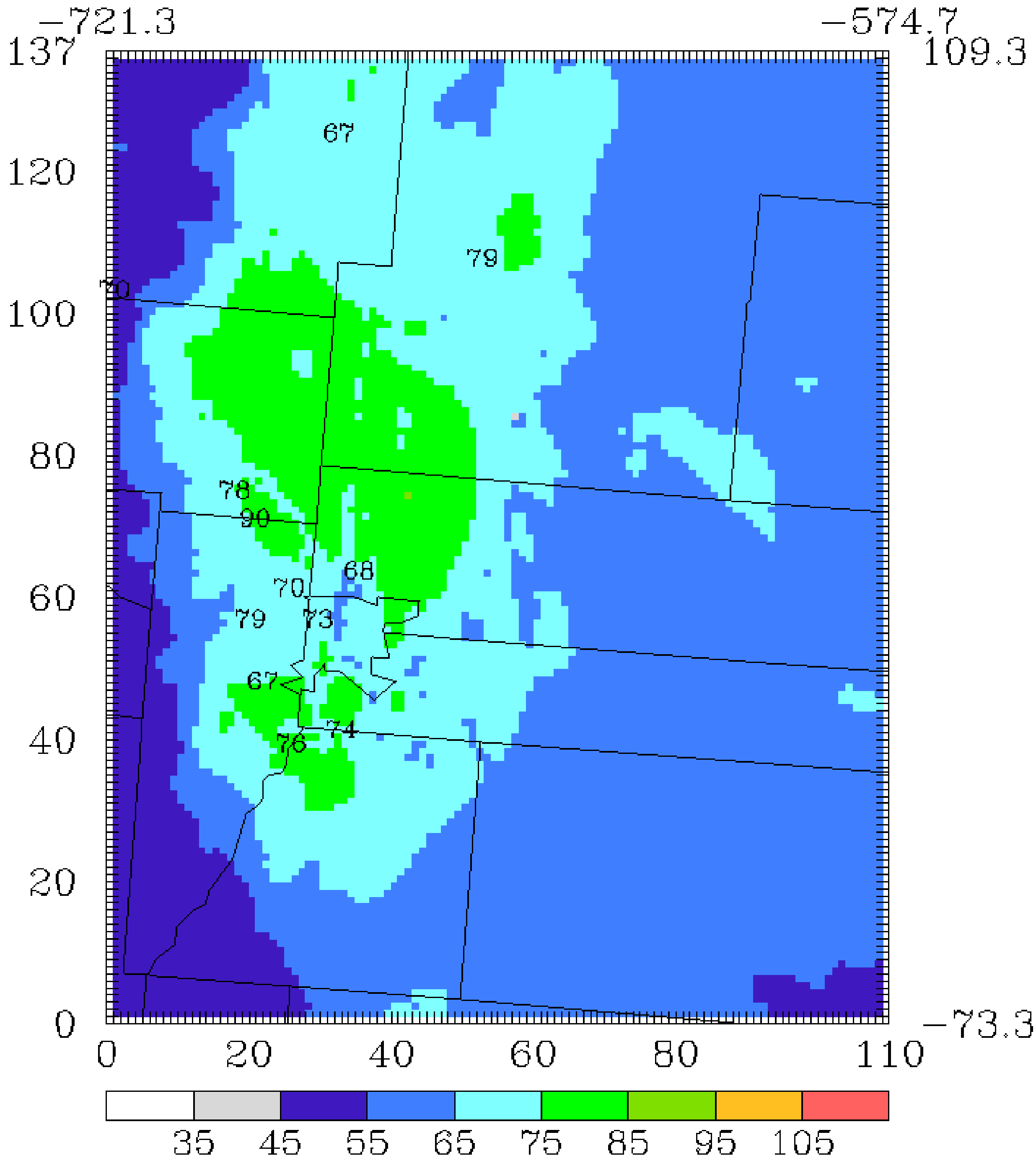


Daily Max. O3 Concentration (ppb)

20020628 : 9999

8 Hour Average

Max value: 8.507E+01 at (43, 75)
Min value: 4.440E+01 at (58, 86) non zero cells only
Avg value: 6.425E+01 non zero cells only
Grid Total: 9.368E+05

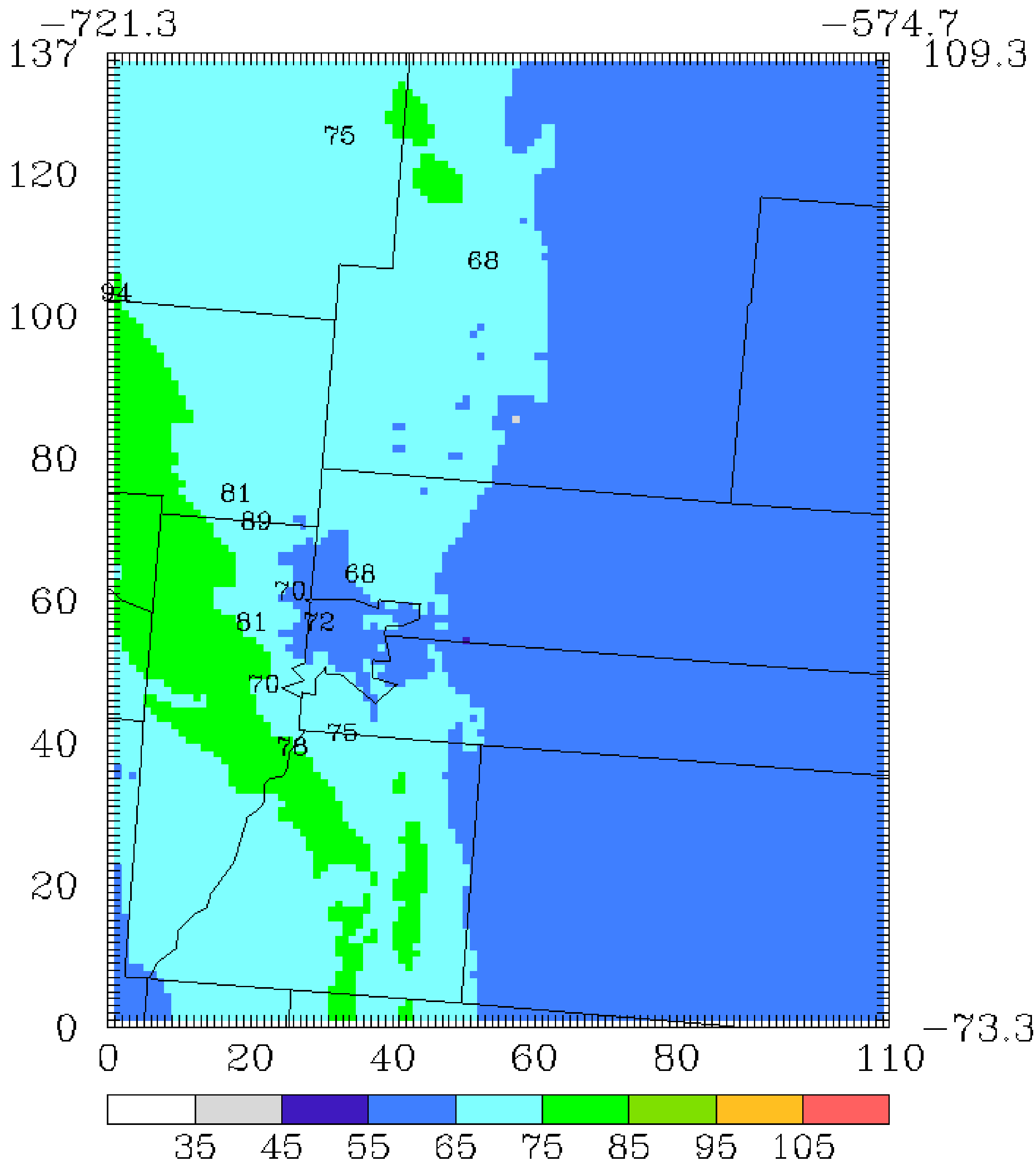


Daily Max. O3 Concentration (ppb)

20020629 : 9999

8 Hour Average

Max value: 8.455E+01 at (23, 38)
Min value: 4.418E+01 at (58, 86) non zero cells only
Avg value: 6.541E+01 non zero cells only
Grid Total: 9.536E+05

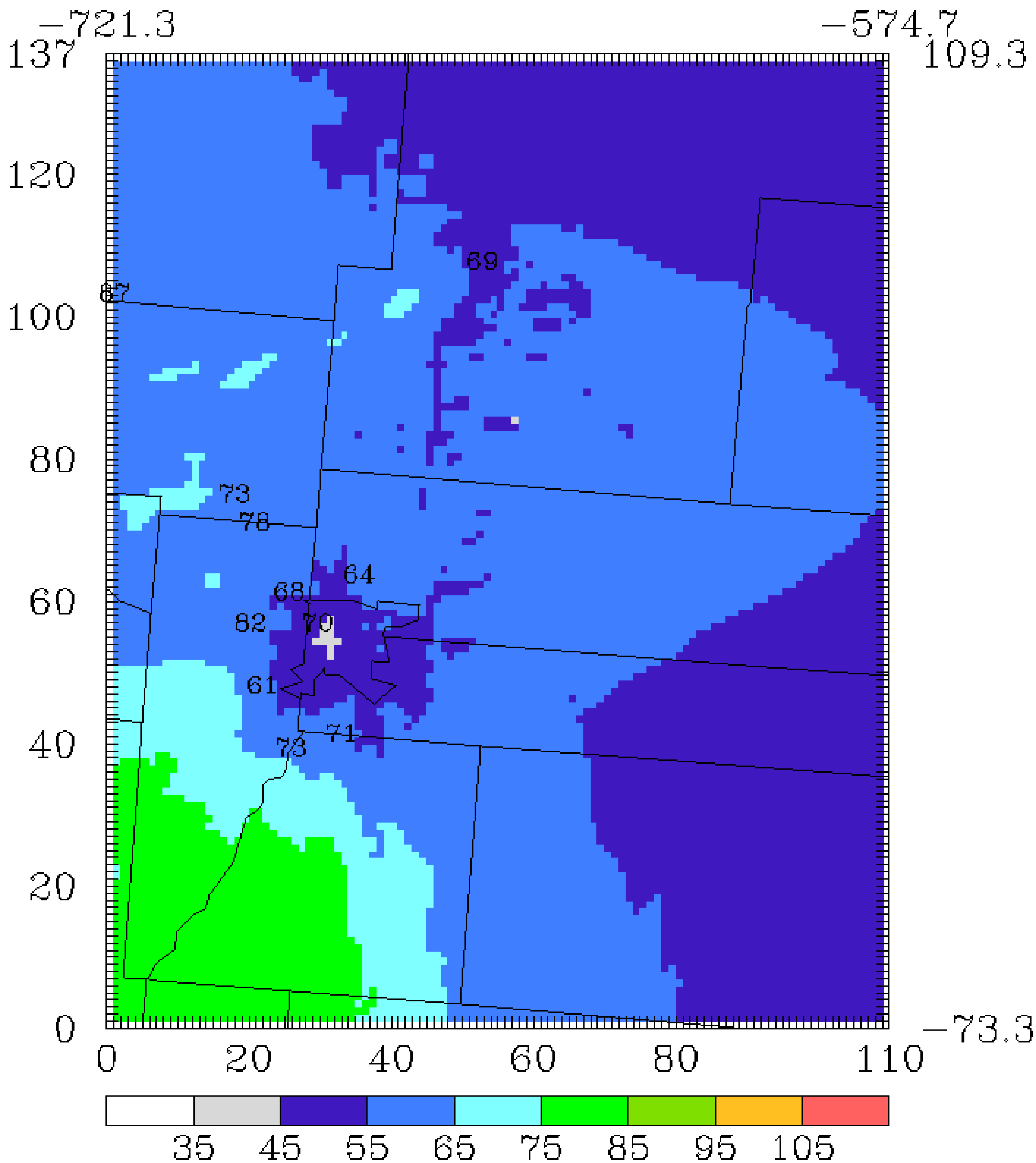


Daily Max. 03 Concentration (ppb)

20020630 : 9999

8 Hour Average

Max value: 8.459E+01 at (31, 9)
Min value: 3.792E+01 at (58, 86) non zero cells only
Avg value: 5.863E+01 non zero cells only
Grid Total: 8.548E+05

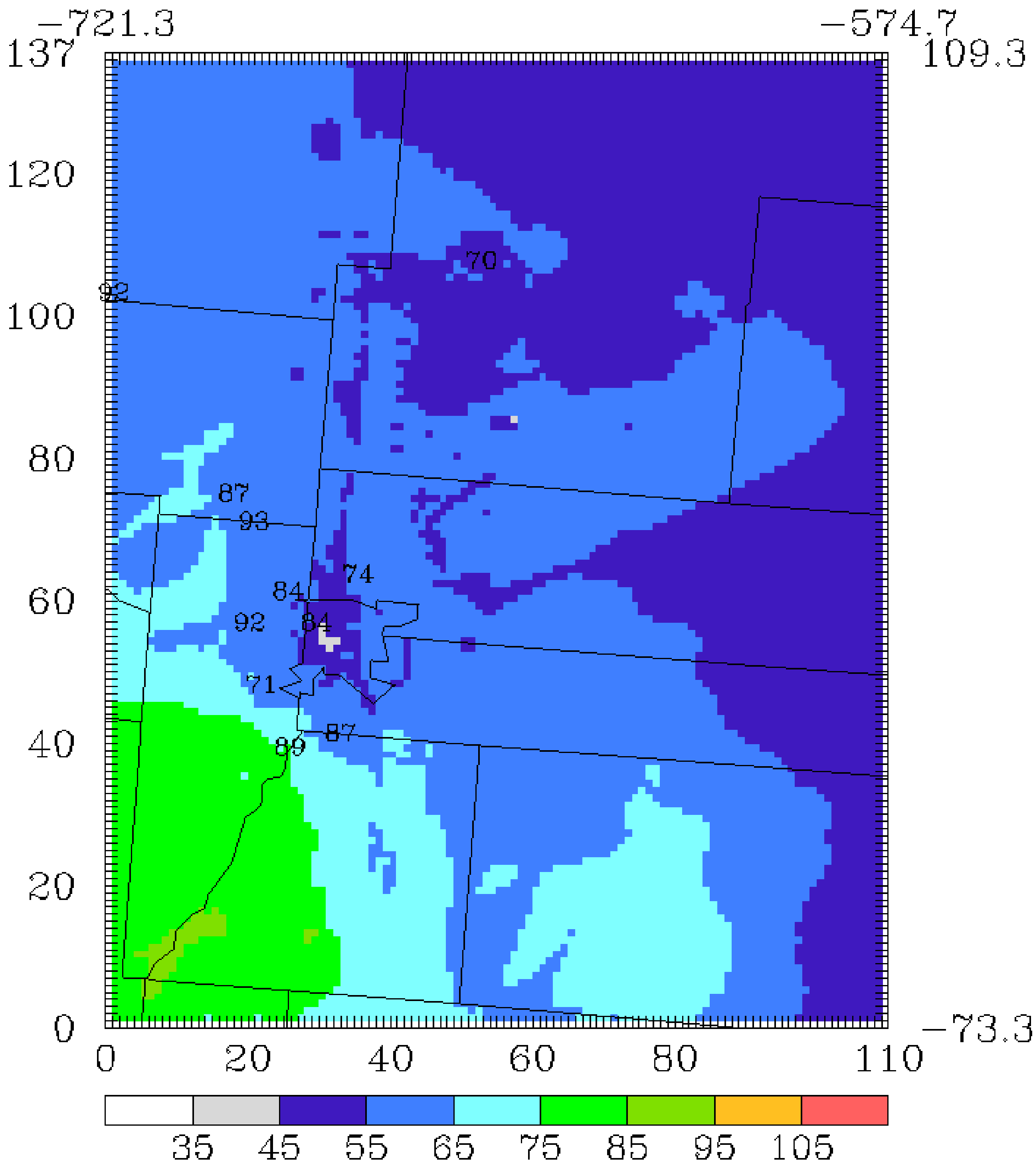


Daily Max. O3 Concentration (ppb)

20020718 : 9999

8 Hour Average

Max value: 8.892E+01 at (8, 8)
Min value: 4.023E+01 at (58, 86) non zero cells only
Avg value: 5.962E+01 non zero cells only
Grid Total: 8.692E+05

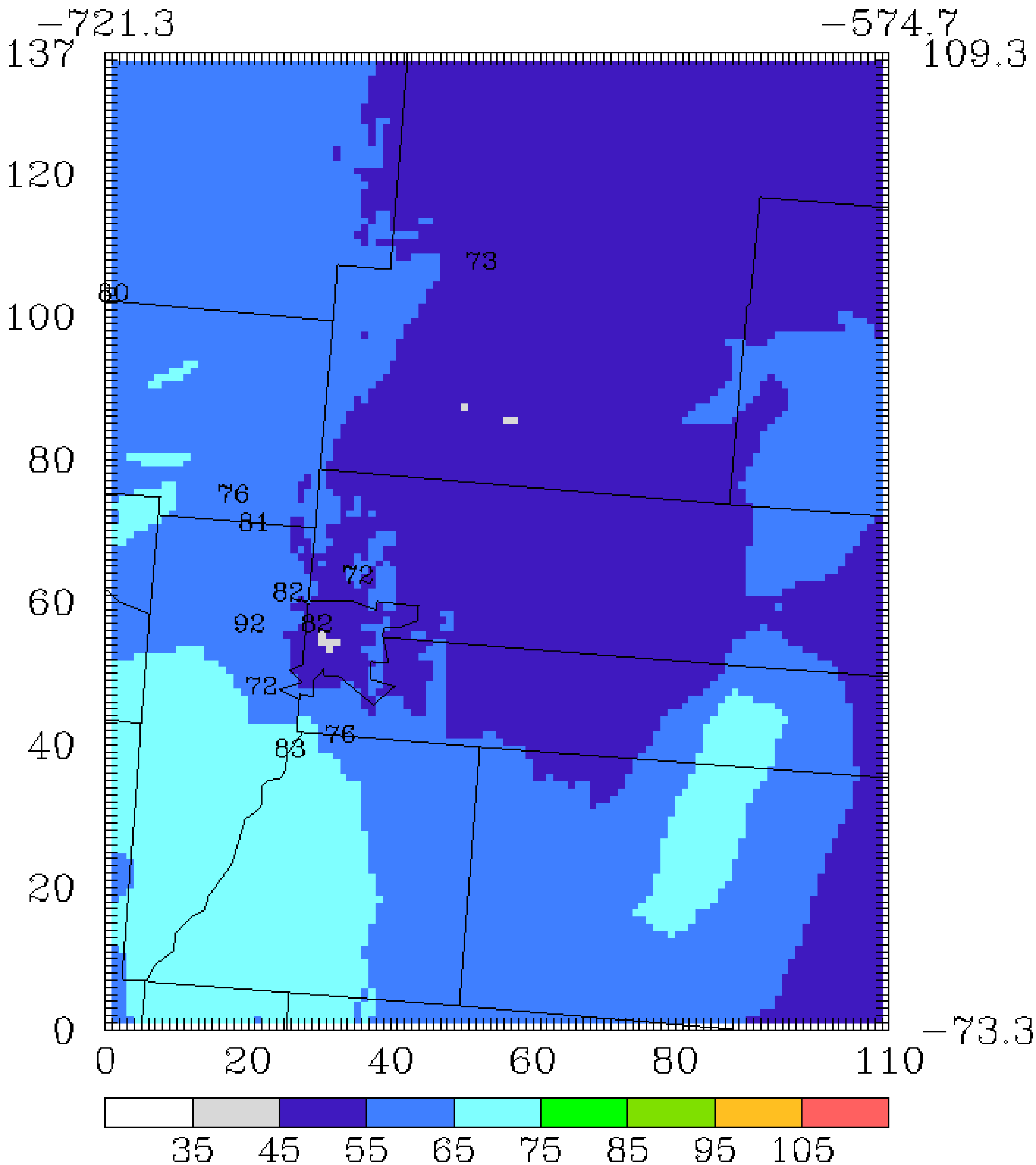


Daily Max. 03 Concentration (ppb)

20020719 : 9999

8 Hour Average

Max value: 7.454E+01 at (20, 40)
Min value: 3.687E+01 at (58, 86) non zero cells only
Avg value: 5.774E+01 non zero cells only
Grid Total: 8.419E+05

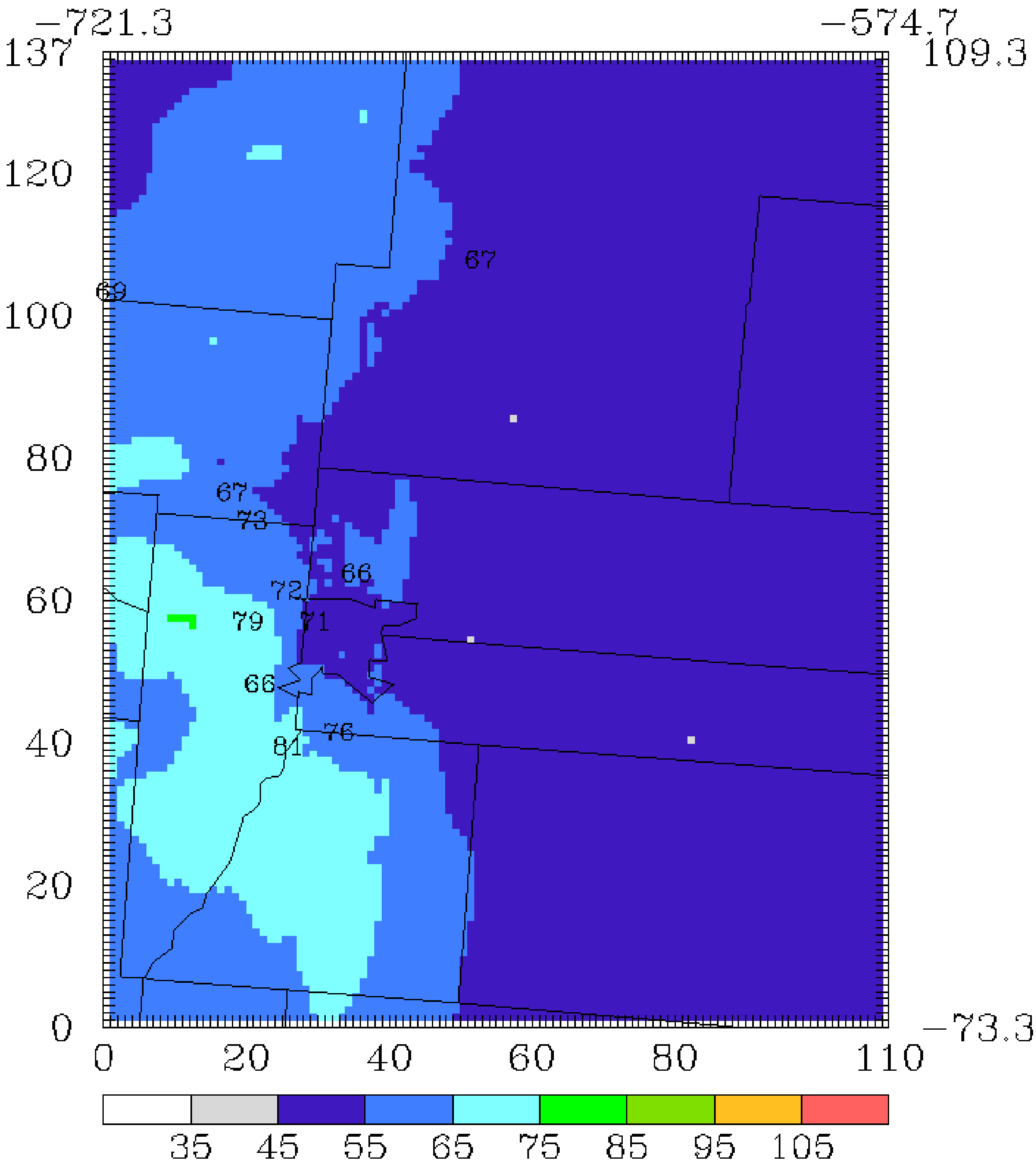


Daily Max. O3 Concentration (ppb)

20020720 : 9999

8 Hour Average

Max value: 7.545E+01 at (13, 58)
Min value: 3.972E+01 at (58, 86) non zero cells only
Avg value: 5.403E+01 non zero cells only
Grid Total: 7.877E+05



Daily Max. 03 Concentration (ppb)

20020721 : 9999

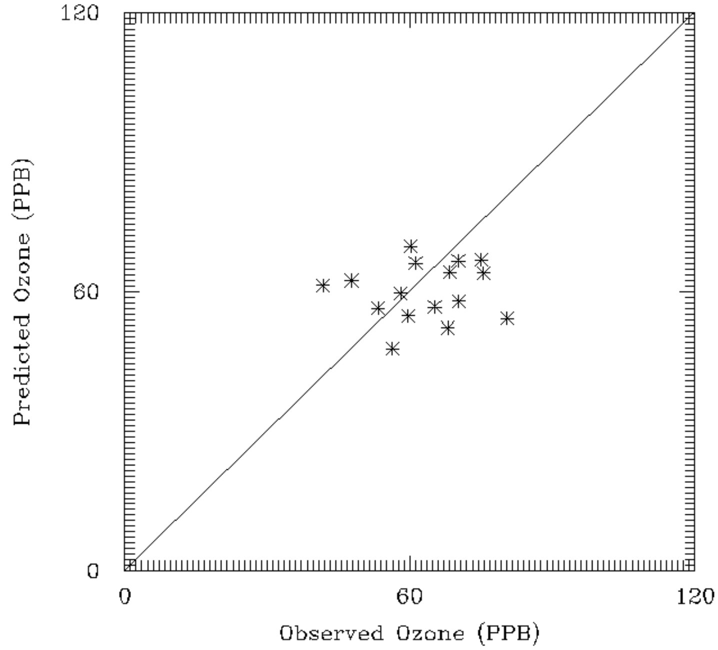
8 Hour Average

Attachment B

Scatter Plot of predicted and observed daily maximum 8-hour ozone concentrations for the Preliminary Base Case simulation on the 4 km grid and:

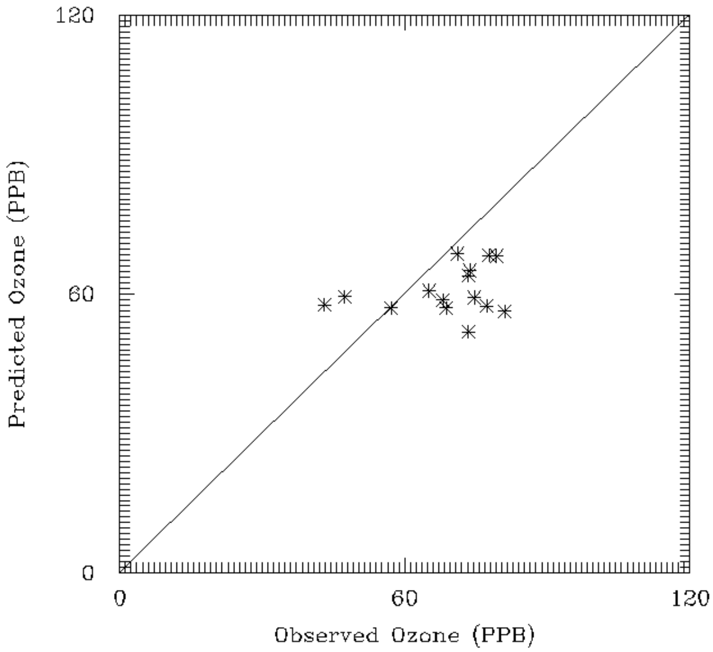
Run 2: June 25 through July 1, 2002 episode
Run 2a: July 18-21, 2002 episode

25 June 2002



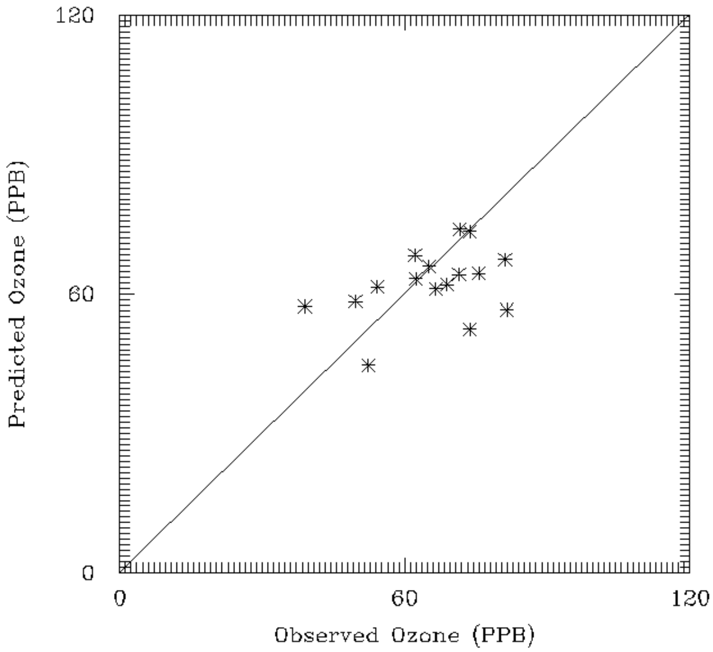
Scatterplot of Daily Maximum Data base1 in the 04

26 June 2002



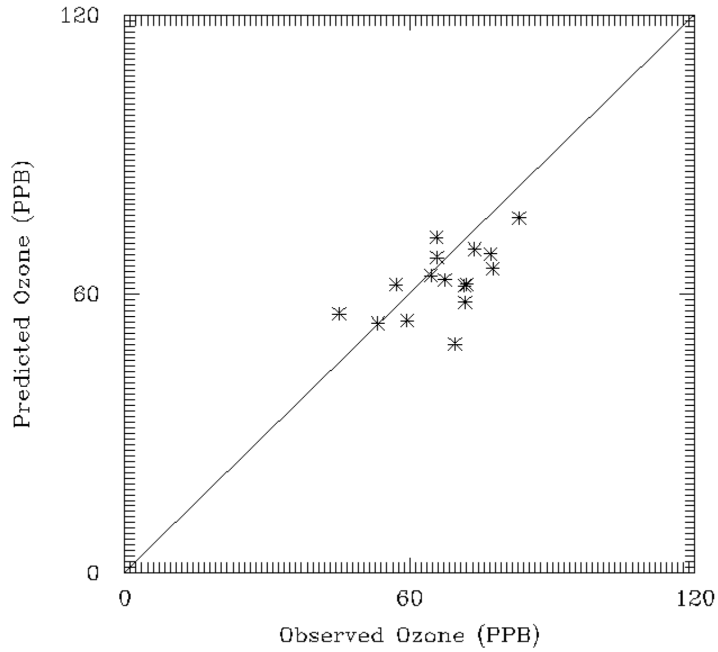
Scatterplot of Daily Maximum Data base1 in the 04

27 June 2002



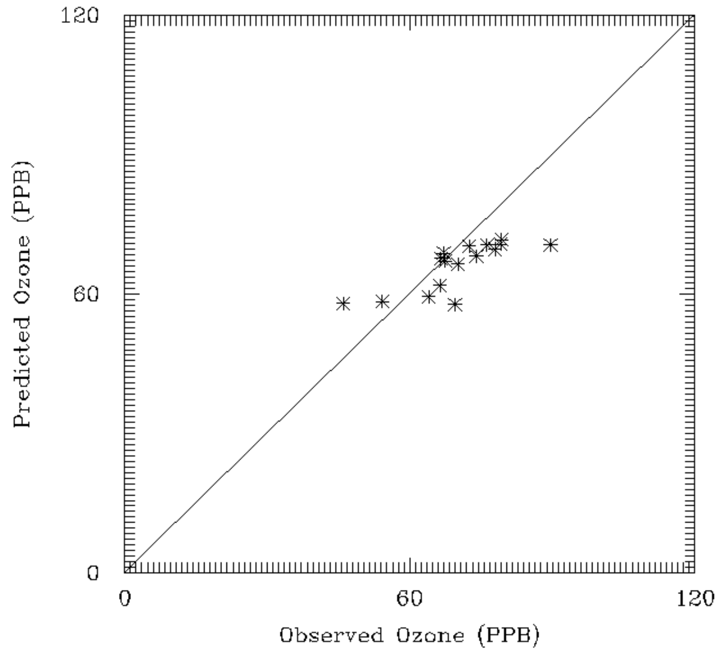
Scatterplot of Daily Maximum Data base1 in the 04

28 June 2002



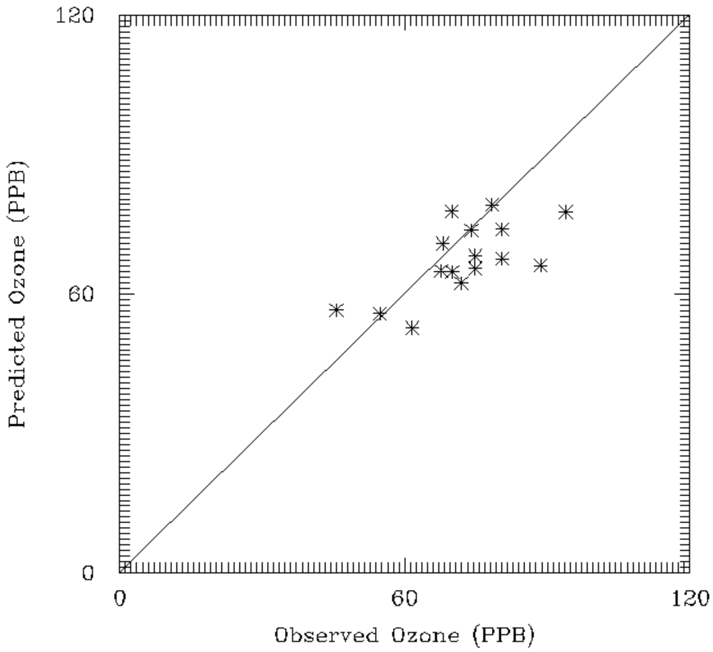
Scatterplot of Daily Maximum Data base1 in the 04

29 June 2002



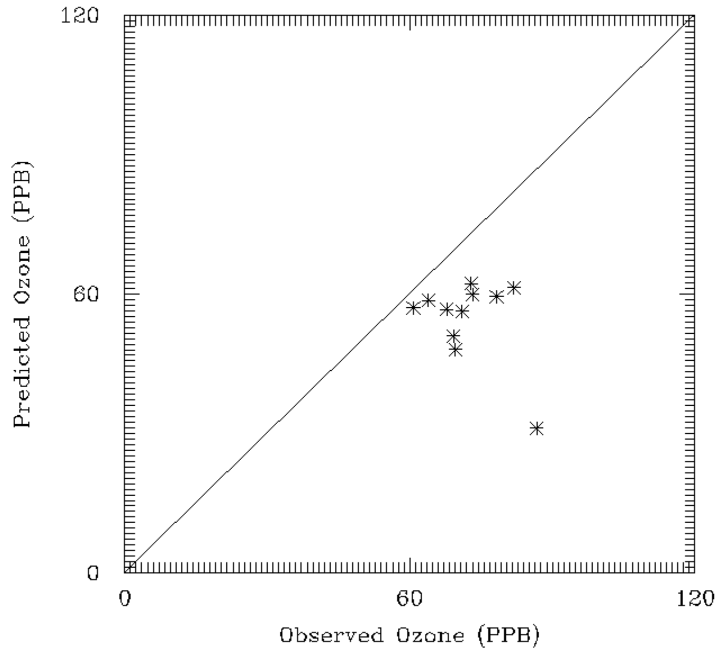
Scatterplot of Daily Maximum Data base1 in the 04

30 June 2002



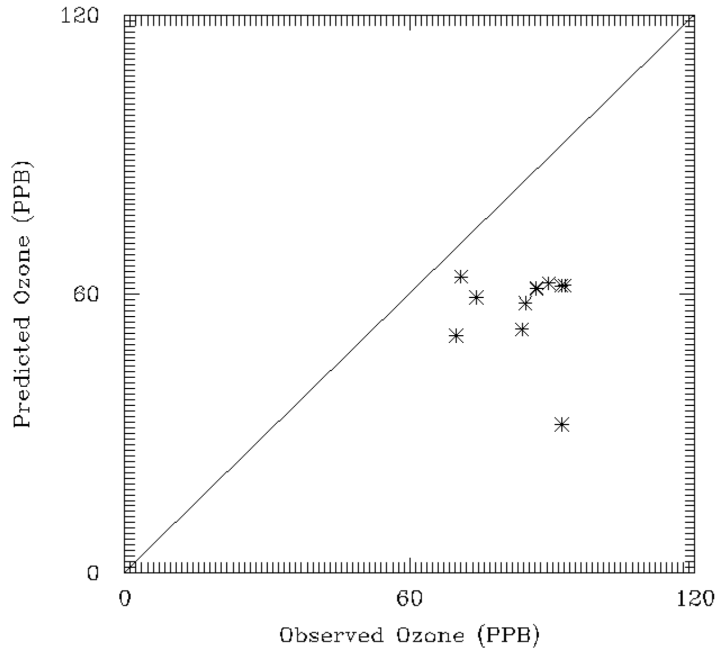
Scatterplot of Daily Maximum Data base1 in the 04

18 July 2002



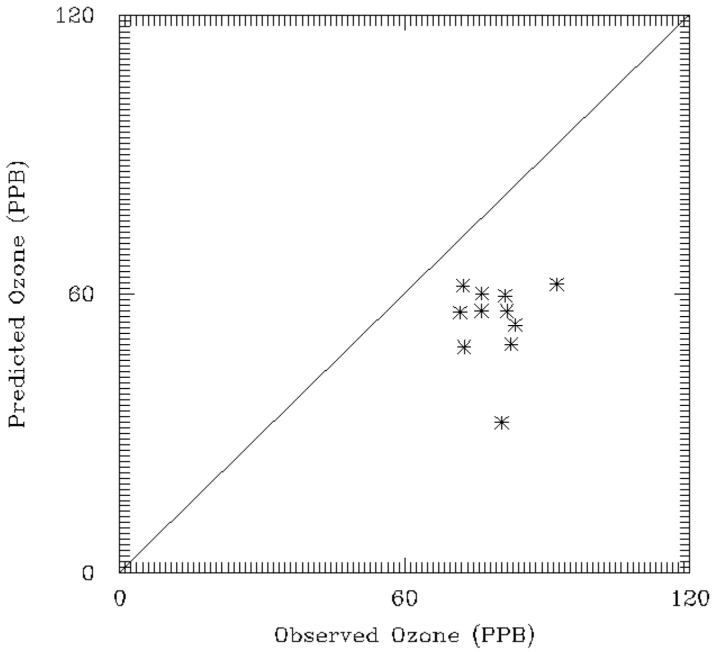
Scatterplot of Daily Maximum Data base1 in the 01.33

19 July 2002



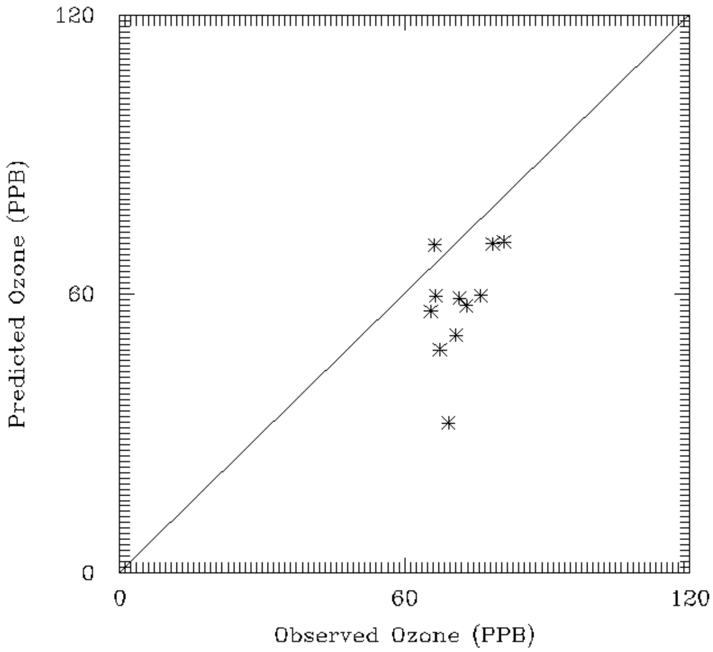
Scatterplot of Daily Maximum Data base1 in the 01.33

20 July 2002



Scatterplot of Daily Maximum Data base1 in the 01.33

21 July 2002



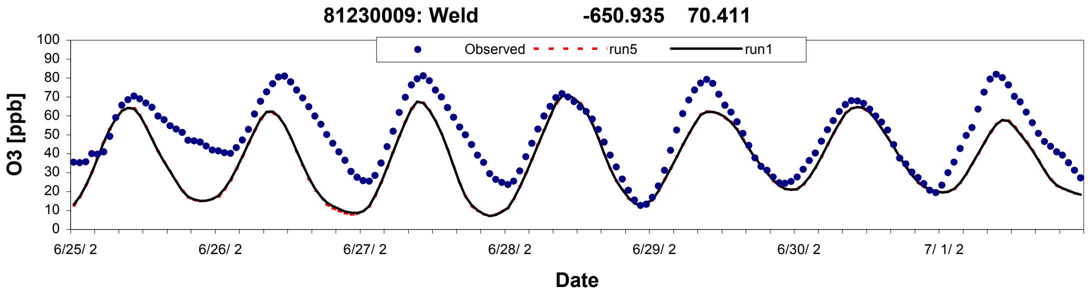
Scatterplot of Daily Maximum Data base1 in the 01.33

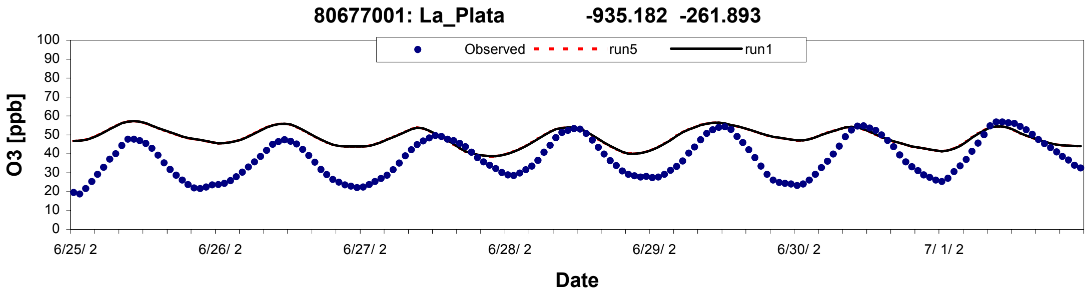
Attachment C

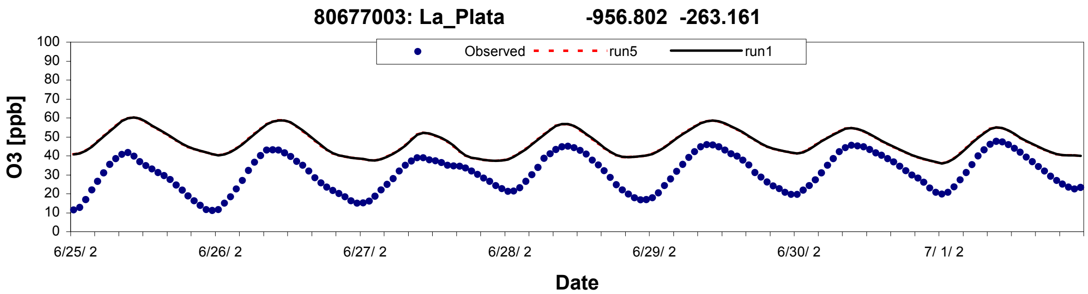
Time Series of predicted and observed 8-hour ozone concentrations
for the Preliminary 36/12 km Base Case (Run 1) and the
Revised 36/12 km Base Case (Run 5) that updates Weld County
Flash emissions: VOC speciation and some Colorado VMT data

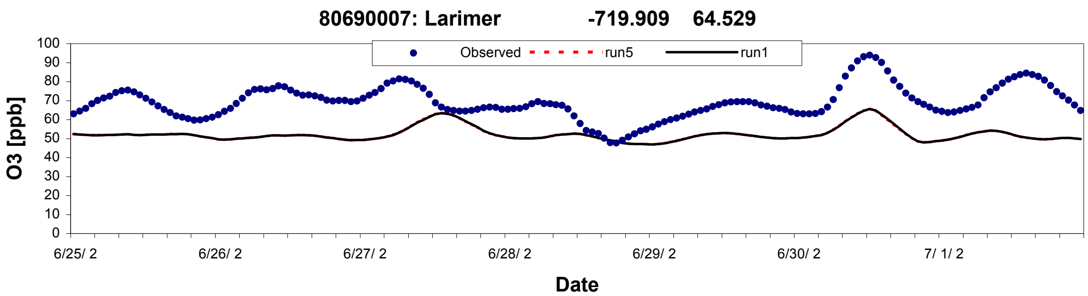
Observed = Dotted Symbols
Estimated Run 2m = Solid Black Line
Estimated Run 2 = Dotted Red Line

Denver Base Case run1 and run5 8hr Ozone 12km

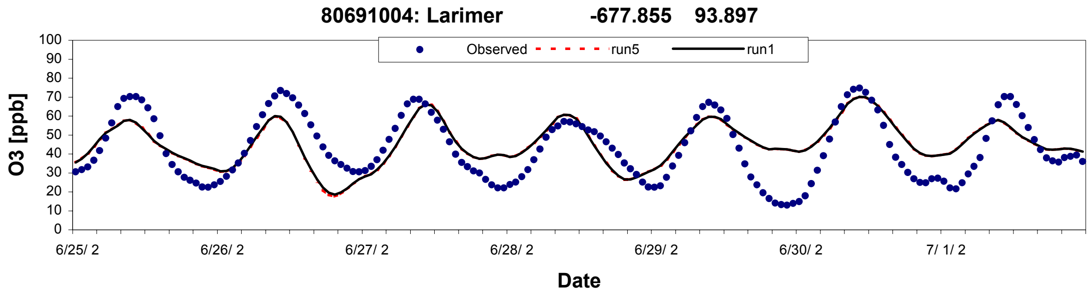


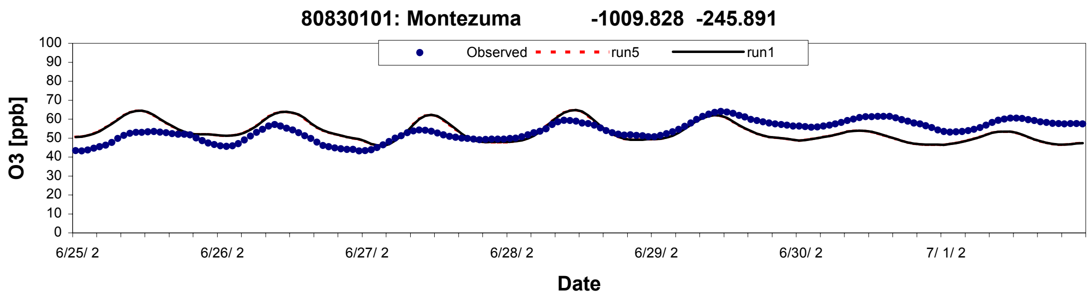


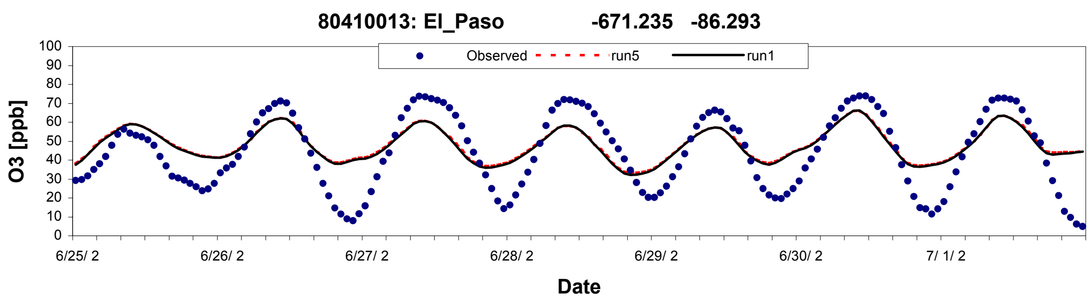


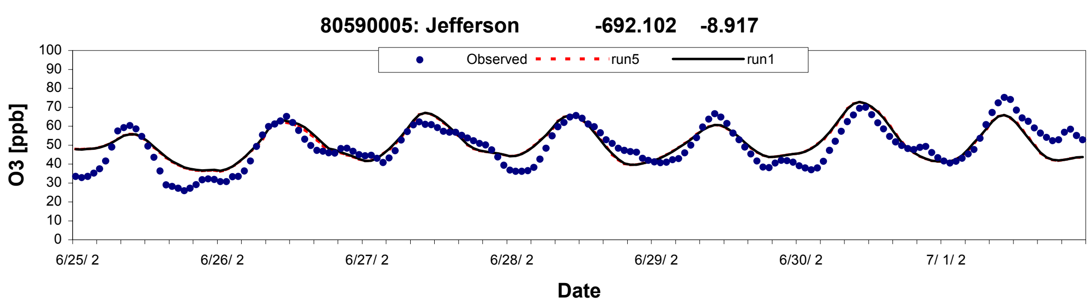


Denver Base Case run1 and run5 8hr Ozone 12km

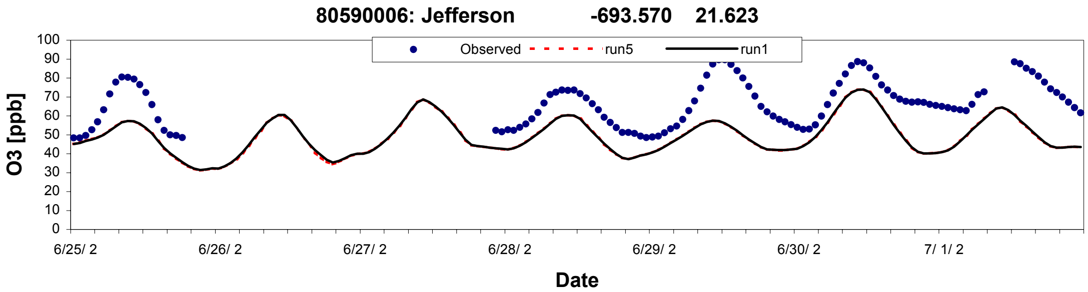


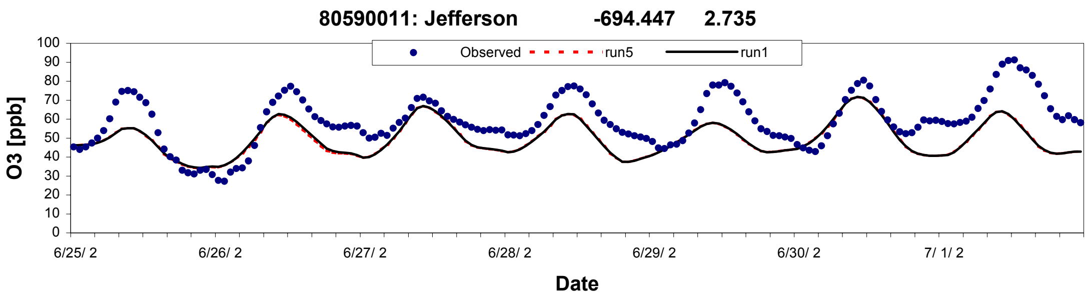


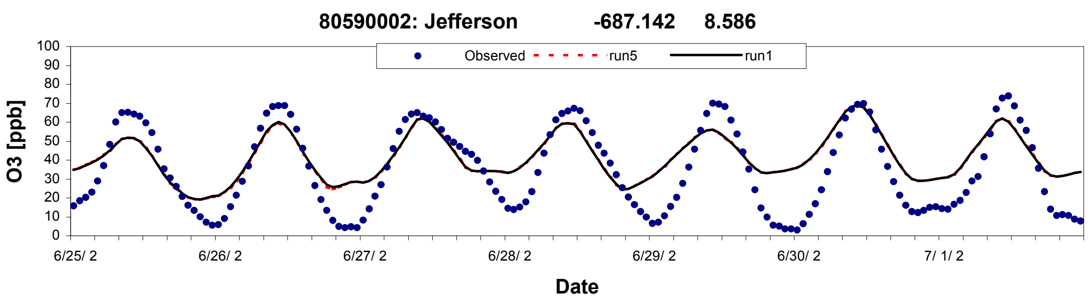


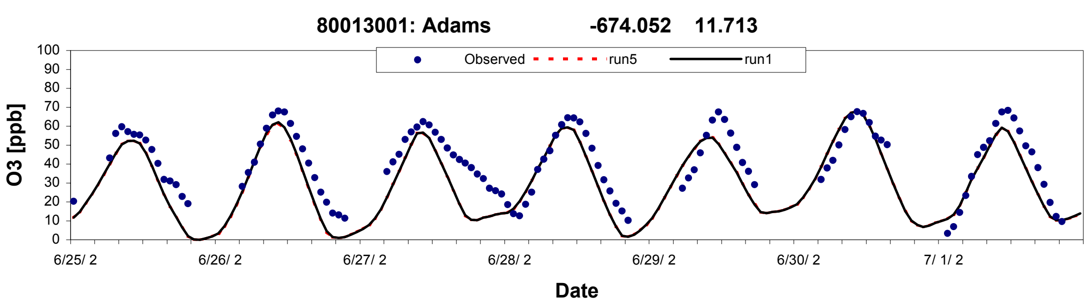


Denver Base Case run1 and run5 8hr Ozone 12km

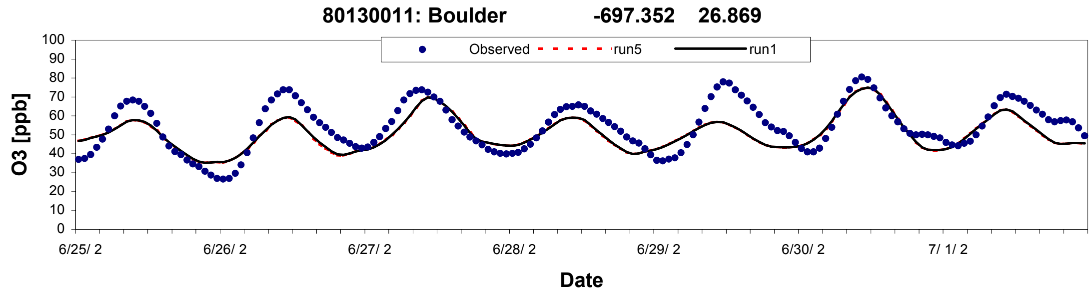


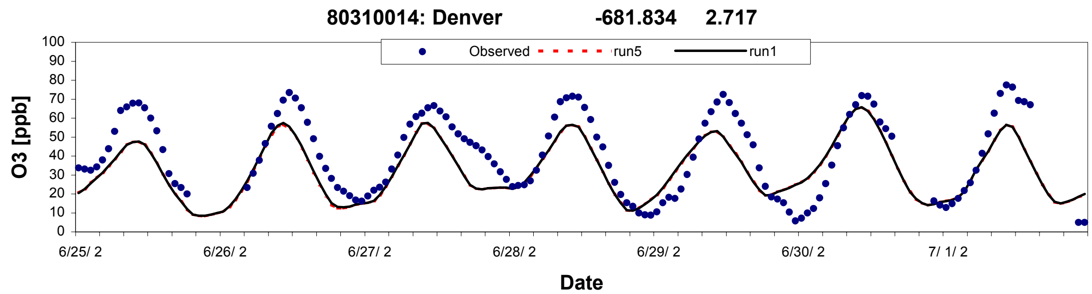


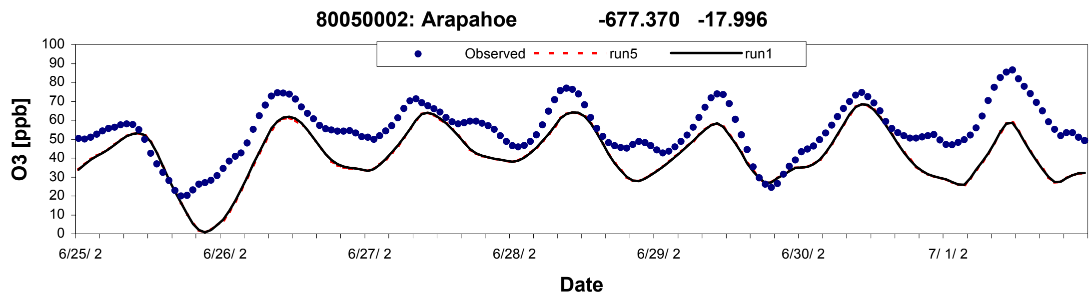


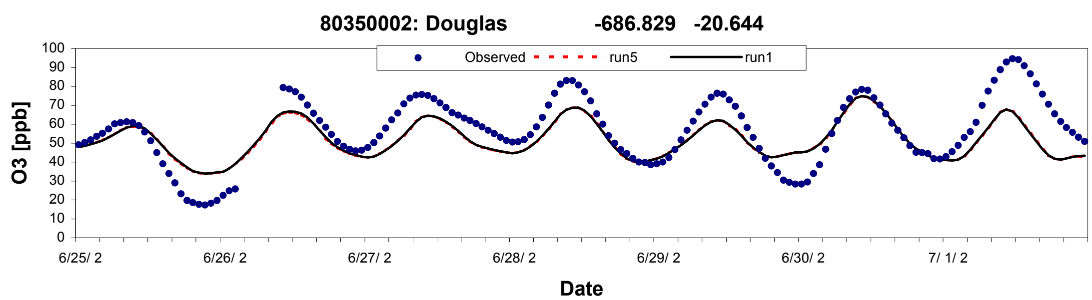


Denver Base Case run1 and run5 8hr Ozone 12km

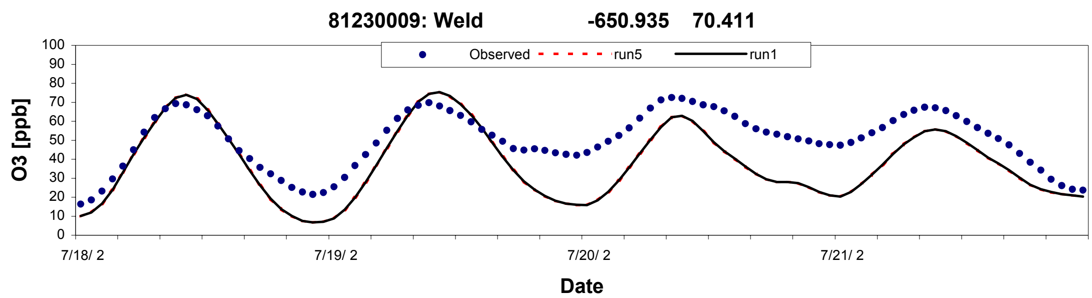


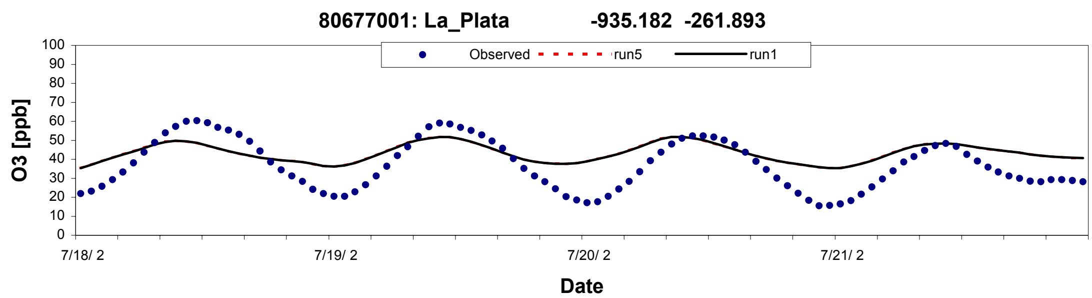


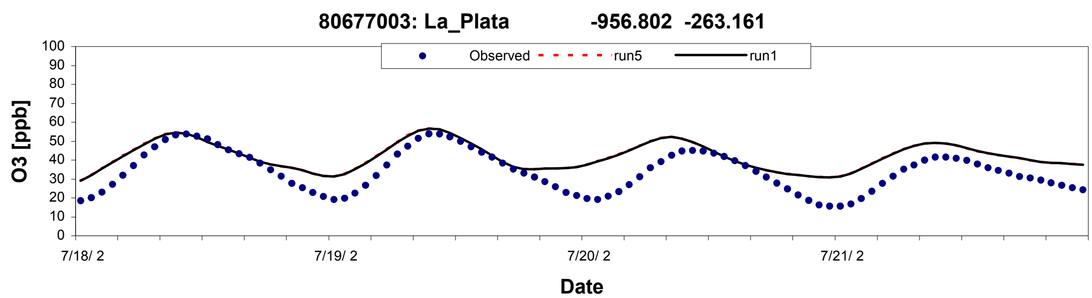


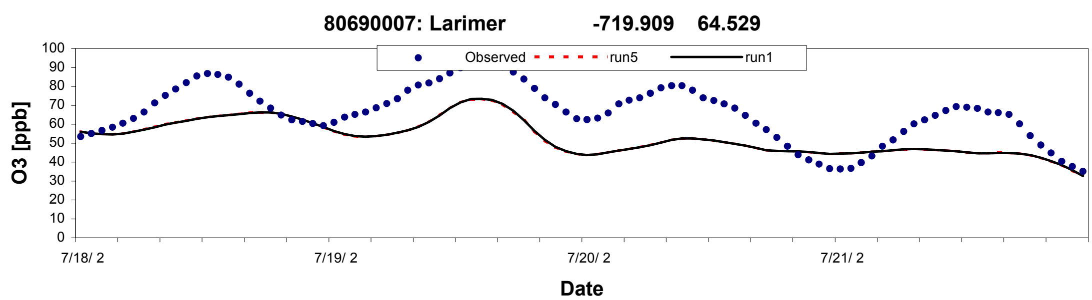


Denver Base Case run1 and run5 8hr Ozone 12km

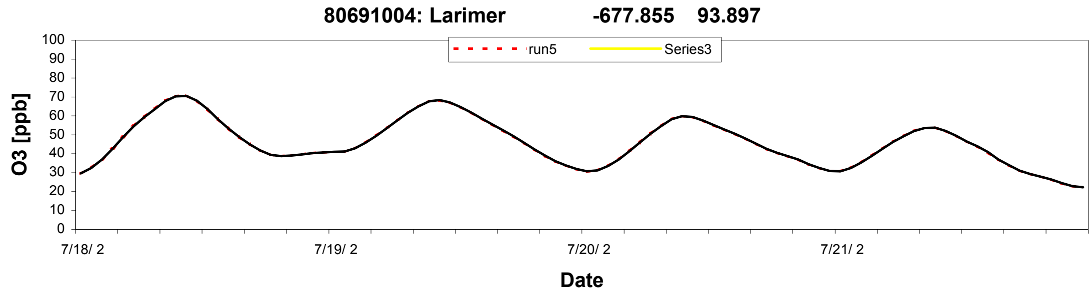


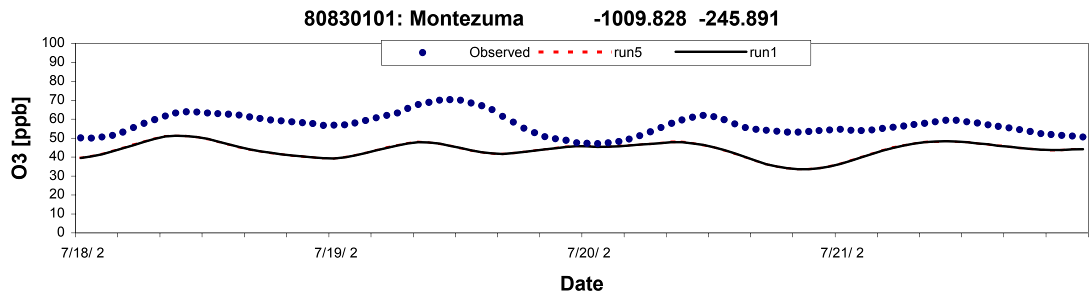


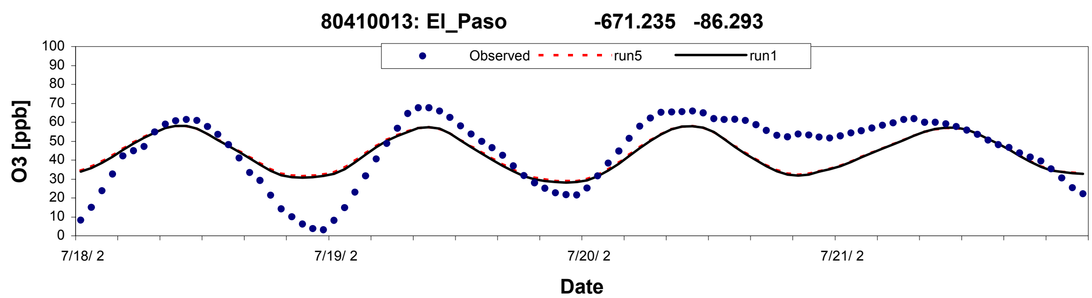


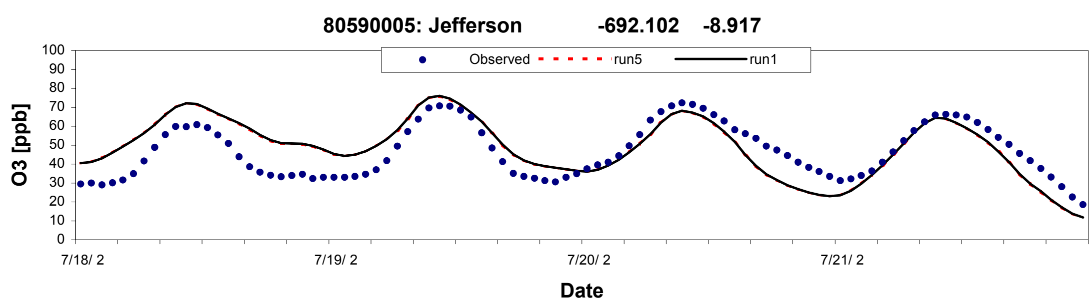


Denver Base Case run1 and run5 8hr Ozone 12km

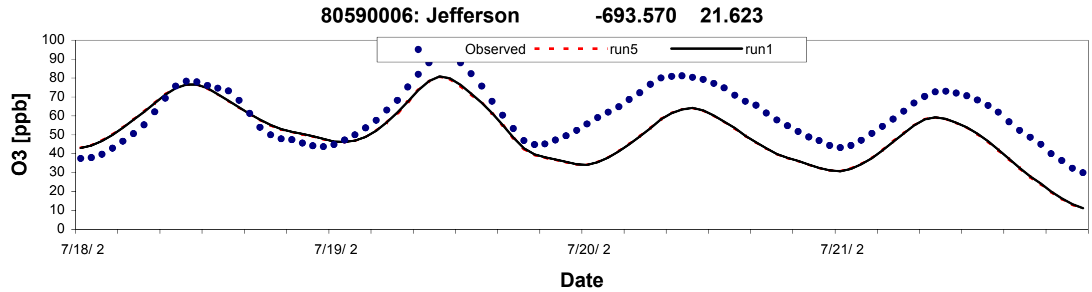


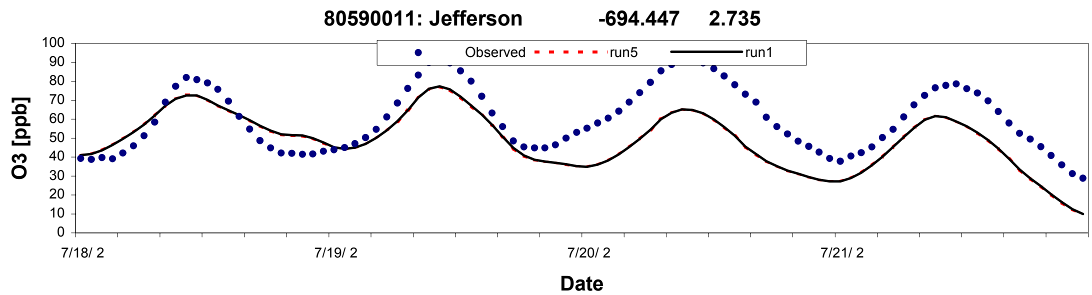


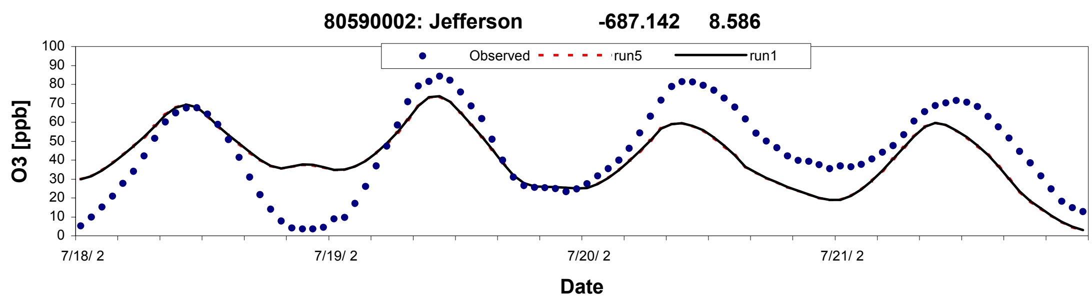


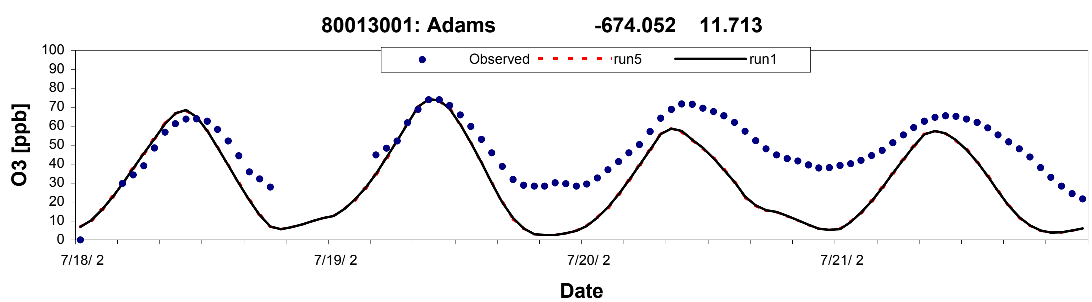


Denver Base Case run1 and run5 8hr Ozone 12km









Denver Base Case run1 and run5 8hr Ozone 12km