APPENDIX E

Evaluation of CAMx Base Case Model Performance for the September 6 - 11, 1993 COAST Episode

HOUSTON/GALVESTON ATTAINMENT DEMONSTRATION - PART II

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EVALUATION OF CAM_X BASE CASE MODEL PERFORMANCE FOR THE SEPTEMBER 6 - 11, 1993 COAST EPISODE

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Table of Contents

1. Introduction 1
2. Statistical Assessment of Model Performance 3
3. Qualitative Evaluation of Model Performance 6
4. Site-by-Site Assessment of Model Performance 12
   4.1 Houston area 12
   4.2 Galveston Bay area 15
   4.3 Beaumont-Port Arthur area 17
   4.4 Southwest Louisiana sites 19
   4.5 Background areas 19
5. Diagnostic Evaluation and Testing 20
   5.1 Effect of Zero Emissions Inventory 20
   5.2 Effect of Alternate Base Year Emissions Inventory 21
   5.3 Effect of Zero Initial and Boundary Conditions 22
   5.4 Effect of Reduced Base Year Wind Speeds 23
6. Conclusions and Recommendations: 24
7. References 25
APPENDIX A - Tables of Model Performance Statistics ..... A
APPENDIX B - Isopleth Plots of Ozone at COAST Monitoring Locations ..... B
APPENDIX C - Time Series Plots of Ozone at COAST Monitoring Locations C
APPENDIX D - Scatter Plots of Ozone at COAST Monitoring Locations ..... D

1. INTRODUCTION

Before an air quality model may used to guide policy decisions on future-year emissions control strategies, the ability of the model to accurately characterize ozone formation must be evaluated. Typically, this is done by comparing the simulated pollutant fields against the ambient observations from a historical ozone episode. This report summarizes the evaluation results from the Comprehensive Air Quality Model with Extensions (CAM_X) over the Houston-Galveston (H-G) region on 6-11 September 1993.

There is quite a bit of history to the photochemical modeling of this Coastal Oxidant Assessment for Southeast Texas (COAST) episode. Initially the variable-grid version of the Urban Airshed Model (UAM-V) was employed to simulate air quality over the region. Model performance was deemed to be satisfactory and an attainment plan for the area was developed. Since then, the Texas Natural Resource Conservation Commission (TNRCC) has decided to switch to the CAM_X model (Environ, 1997), so that all modeling data and software can be made available to the regulated community. Additionally, the base case biogenic inventory was revised to better reflect actual emissions from non-anthropogenic sources. The following list summarizes the pertinent information from the earlier studies.

- Based on United States Environmental Protection Agency (USEPA) model evaluation criteria, the initial UAM-V modeling was statistically acceptable (TNRCC, 1998a).

- Only one day failed to meet the USEPA criteria. The ramp-up day of 7 September exhibited and unpaired peak accuracy of 39.4 percent (TNRCC, 1998a).

- The model was unable to replicate the highest episodic observed ozone values (> 210 ppb) recorded on 8 September (TNRCC, 1998a).

- The CAM_X simulation results were slightly higher on average (3-7 ppb) than their UAM-V counterparts when the same input data sets were used. This resulted in slightly higher positive bias (overprediction) in the CAM_X modeling, although the statistics continued to reside within USEPA recommended ranges (MCNC, 1999a).

- Revising the base-year biogenic inventory did not significantly alter CAM_X ozone predictions on a domainwide scale. Simulated ozone concentrations in Houston were 5-15 ppb lower with the incorporation of the revised biogenic estimates (MCNC, 1999b).

According to prevailing thought in the air quality modeling community, it is possible to separate a meaningful model performance evaluation into two components (Tesche, 1990):

1. the *operational evaluation* which consists primarily of comparisons between the model and observed data, both qualitative and statistical, and

2. the *scientific evaluation* which attempts to determine if the physical processes leading to ambient pollutant concentrations are represented properly in the model.

This assessment of CAM_X model performance over the 6-11 September 1993 episode consists mostly of an operational evaluation because of a) the wealth of model performance information already prepared for the previous base cases, b) CAM_X version 1.13 is not equipped with process analysis which facilitates such a scientific evaluation, and c) a paucity of ambient data aloft and schedule constraints work against a rigorous model evaluation.

Several other measures, however, were taken to ensure the highest possible quality model output fields. At each step prior to conducting base case simulations, the input fields were quality assured for consistency and obvious errors. Additionally, several diagnostic tests were completed to check the model formulation and response to various inputs. The goal of diagnostic testing is to determine whether a model exhibits expected behavior under extreme changes to its input. Diagnostic tests check for spurious behavior that might indicate problems in the model formulation. The results of the five diagnostic simulations are summarized in Section 3 of this report.

As outlined in the modeling protocol (TNRCC, 1998b), several methods were used to assess the model precision in reproducing observed ozone over the September 1993 episode. Statistical methods can provide a quantitative measure of model performance. The results of these methods must be considered carefully, especially in cases where there are not a large number of monitors. Graphical displays comparing predicted to observed concentrations can provide qualitative information on model performance. The following techniques will be used in this analysis:

- Unpaired Peak Accuracy: This measure calculates the difference between the highest observed value and the highest predicted value independent of time and space. (USEPA recommended range: $\pm$15-20%)

- Normalized Bias: This test measures the ability of the model in reproducing observed patterns. Since there are many time periods when relatively low levels of ozone are predicted, and statistics from these periods are not very meaningful, this test will be limited to pairs where the observed concentration is greater than 60 ppb. (USEPA recommended range: $\pm$5-15%)

- Gross Error: This test will compare the difference between all pairs of predictions and observations that are greater than 60 ppb. This is a measure of model precision. (USEPA recommended range: 30-35%)

- Time-Series Plots: For each monitoring station in the domain and for each hour in the episode, the predicted concentration will be compared with the monitored concentration. This will determine if the model can predict the peak concentrations and if the timing of ozone generation in the model agrees with that found with the monitoring. Because modeled volumetric concentrations are compared with data from monitoring sites, that are specific

points in space, it should not be expected that agreement would be excellent.

- Surface-Level Isopleths: For selected daytime hours, surface-level isopleths (lines of equal concentration) will be drawn. This shows how the model is predicting the extent, location, and magnitude of ozone formation. This information can be compared to monitoring results.

- Scatter plots: Scatter plots of predictions compared to observations depict the extent of bias in the ensemble of hourly data pairs. Systematic positioning of data points around the perfect correlation line indicates bias. The distribution of points over the area is an indication of error.

2. STATISTICAL ASSESSMENT OF MODEL PERFORMANCE

When viewing these results, remember that CAMx predicts a volumetric one-hour average over an entire grid cell. Monitoring data provides a measure of air quality at a specific point in space. To provide an accurate comparison with model predictions, the monitoring data would have to be transformed into volumetric one-hour averages over the same grid cells used in CAMx. However, monitoring networks are not dense enough to provide this information even for the most intensive studies that have been performed. Thus, comparison between the CAMx volumetric predictions and the monitored point measurements are the only recourse. This can provide insight into the model prediction accuracy, but does not provide precise measures of model performance. Also, since the two days of each modeling episode are initialization days during which ozone exceedances were not recorded, performance measures will be applied only to modeling results subsequent to the ramp-up days.

Table 1 displays some of the first-order evaluation statistics generated from the H-G 1993 base case as calculated over the entire domain. The statistics do not consider observed-model pairs where the observation is less than 60 ppb. As can be seen from the table and Figure 1a, model performance for the COAST September 6-11, 1993 episode

Date	Max Model Ozone Domainwide (ppb)	Max Model Ozone Stationwide (ppb)	Max Obs Ozone (ppb)	Unpaired Peak Accuracy	Normalized Bias	Normalized Gross Error	Mean Simulated (ppb)	Mean Obs (ppb)
9/6/93	164.2	125.8	136	.207	.127	.199	82.5	73.9
9/7/93	167.4	118.1	111	.508	.125	.196	80.3	72.1
9/8/93	**181.9**	**169.9**	**214**	**-.150**	**.120**	**.242**	**99.5**	**91.8**
9/9/93	**179.6**	**163.0**	**195**	**-.079**	**.112**	**.239**	**94.6**	**87.2**
9/10/93	**177.8**	**166.6**	**162**	**.097**	**.002**	**.226**	**89.2**	**91.0**
9/11/9	**185.6**	**143.9**	**189**	**-.018**	**.108**	**.224**	**94.8**	**88.6**

3								

Table 1. Model performance statistics. Values in bold are for the primary episode days. meets the criteria outlined by USEPA for an acceptable base case. The unpaired peak predictions exhibit a negative (underprediction) bias on all days but the 10th and range from to 2 to 15 percent. While the maximum ozone is generally underpredicted, the mean ozone greater than 60 ppb is overestimated in the model. Normalized bias values range from near zero on the 10th to 12% on the remaining episode days. Gross error is fairly consistent at around 23 percent.

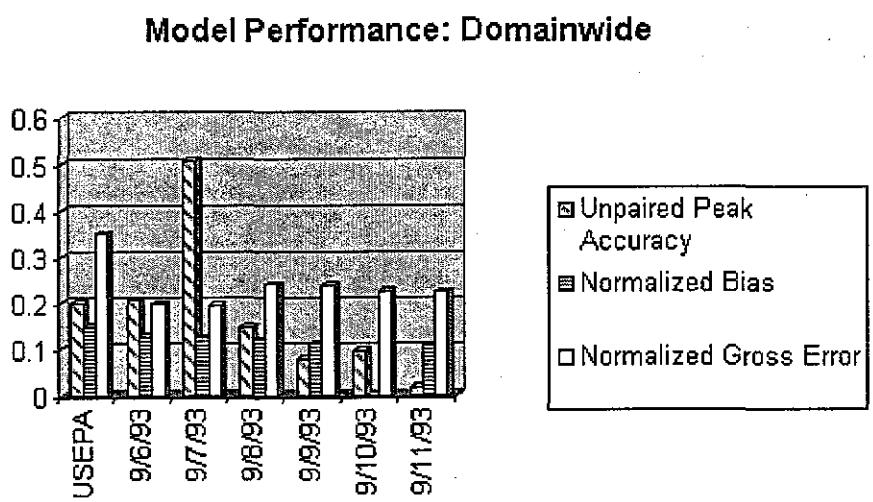

Figure 1a. Comparisons of COAST CAMx domainwide performance statistics against USEPA recommended bounds. Absolute values were used for all criteria to simplify plot.

These calculations were also made looking specifically at the nonattainment subregions (H-G[1], and Beaumont-Port Arthur[2]). Figures 1b and 1c show the results. With the exception of the normalized bias on 8 September in the Beaumont-Port Arthur (B-PA) region, all statistical criteria indicative of adequate model performance are met. The overprediction on the 8th in the Beaumont region is due to a deficiency in the meteorological fields. Within the model, a large amount of ozone is advected into the region from the Gulf of Mexico via a model sea breeze that is initiated, within the model, around midday on the 8th. Appendix A provides the complete performance tables for each day of the episode and all three regions.

[1] Includes all monitors in Harris, Galveston, Chambers, and Brazoria counties.
[2] Includes all monitors in Orange, Jefferson, and Hardin counties.

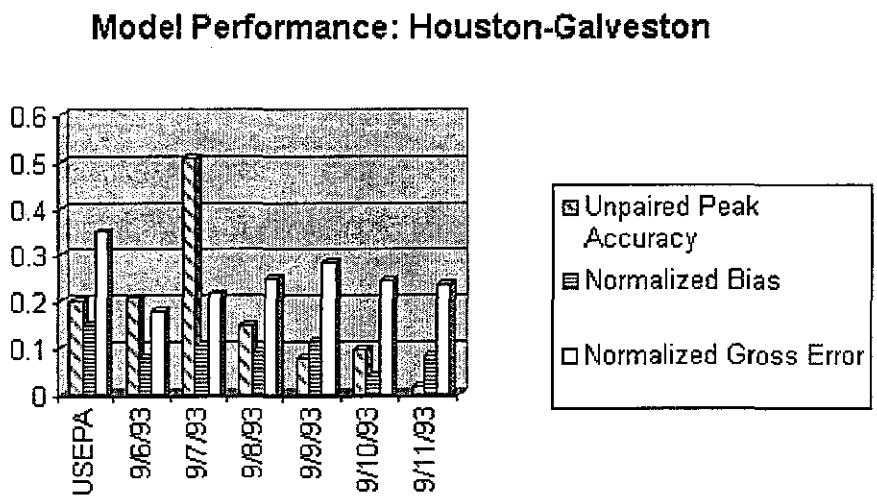

Figure 1b. Comparisons of COAST CAMx performance statistics in Houston-Galveston nonattainment counties against USEPA recommended bounds. Absolute values were used for all criteria to simplify plot.

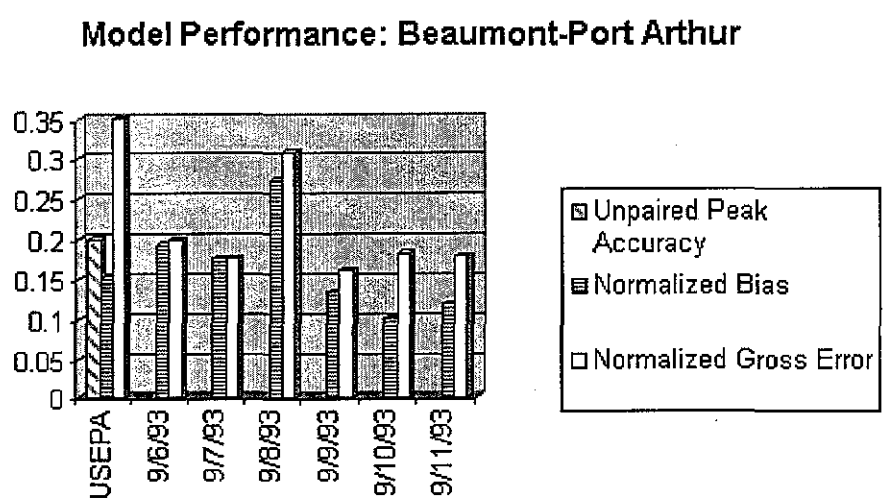

Figure 1c. Comparisons of COAST CAMx performance statistics in Beaumont-Port Arthur nonattainment counties against USEPA recommended bounds. Absolute values were used for all criteria to simplify plot. Unpaired peak accuracy is not considered in this case as the model and observed peaks were in the Galveston Bay region.

3. QUALITATIVE EVALUATION OF MODEL PERFORMANCE

Figure 2 displays a scatter plot of model-observed pairs for all hours of the September 1993 episode. Generally, the performance of the CAMx COAST modeling for this episode is comparable to many other photochemical modeling exercises. In particular, the inability of the model to reproduce the highest ozone levels at specific sites is a feature often seen in this type of modeling. While underestimating the (relatively limited) highest ozone concentrations, the model tends to overestimate observations in the 60-80 ppb range. This leads to the overall positive bias seen in the performance statistics and is also not uncommon in modeling applications such as this.

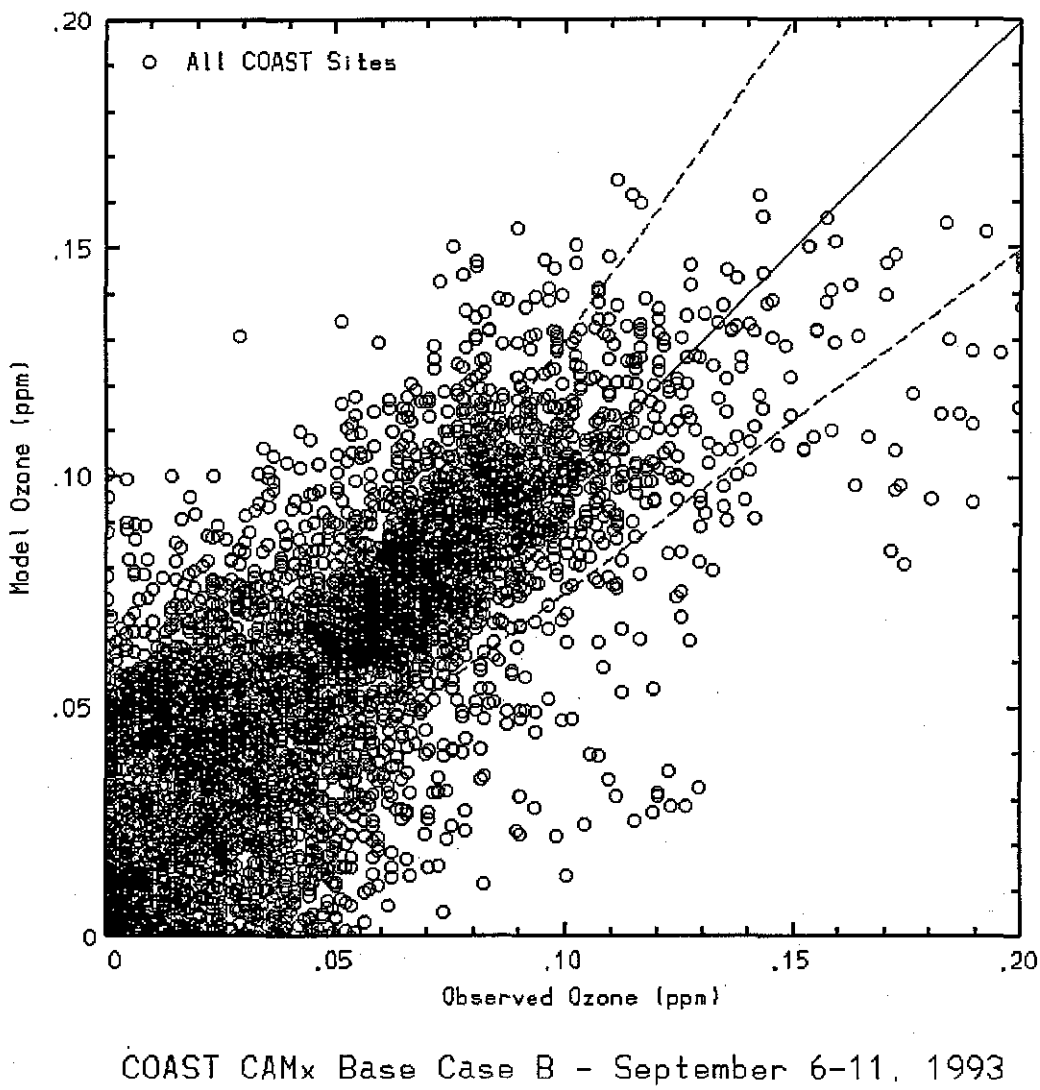

Figure 2. Scatter plot of ozone observations vs. model ozone for the September 1993 COAST episode. Pairs were generated for all hours and monitoring data points. The solid line represent non-biased model predictions. The dashed lines bound a region of acceptable model bias.

Appendix B contains model isopleth plots with overlaid observations for 1000, 1200, 1400, 1600, 1800, and 2000 CST for each day of the episode. These plots allow for a limited evaluation of the spatial accuracy of the base case simulation results. Descriptions of the qualitative differences between the afternoon observed and model fields follow.

Observations on the afternoon of the 1st day of the episode are relatively low. Most sites in Houston record values in the 70 ppb range. The exception to this rule is the HSMA site in southern Harris county that is at 93 ppb. There are also some higher values (low 90s) in Jefferson county. The model accurately predicts the relatively low ozone over Houston on the 6th. Additionally, the model indicates a large ozone plume downwind of Houston in Fort Bend county that is consistent with the HSMA monitor, but impossible to validate due to a lack of ambient data. The model does generate an area of 100-110 ppb ozone in Jefferson county, but as this plume is not over any one particular monitor it is hard to verify whether the model ozone production is overdone or not. Finally, the model generates a significant ozone plume (~ 125 ppb) downwind of Lake Charles LA that is not consistent with the ozone values in that region. Though again, the model plume is not co-located with a monitor.

Ozone is very low in Houston of 7 September with most sites in the 40-50 ppb range. Ambient ozone values increase south of Houston, for example HSMA recorded 87 ppb, the Brazoria county site near Clute, TX recorded 92 ppb, and the Victoria and Corpus Christi sites were all in the 80s. The B-PA and Louisiana sites are also low on the 7th, approximately 60 ppb. The model captures the dominant feature of the day's ozone, that is, all of the high values are in the southern part of the domain. Based on the Corpus Christi data (only 2 points) it would seem that the magnitude of the Houston plume is overestimated or transported too far downwind in the modeling. The B-PA and Louisiana region is modeled fairly accurately.

Figure 3 shows the observation and modeled ozone fields at 4 p.m. on 8 September. Very high levels of ozone were detected on this day, particularly in the Galveston Bay region. The Seabrook and Smith Point monitors recorded 208 and 183 ppb, respectively, at this hour. The region of high ambient ozone extended a short distance into Houston where sites east of the city observed values from 100-130 ppb. The further from Galveston Bay, the lower the ozone was. Sites just west of the city observed ozone in the 80s. Interestingly, the monitor in Galveston was also relatively low on this day (~ 80 ppb). Values in the B-PA region ranged from 60-80 ppb.

An encouraging aspect of model performance on this day is that the CAMx results show the sharp ozone gradient between Galveston Bay and Houston. Additionally, while the model does not reproduce the 208 ppb observation at Seabrook it does simulate values as high as 182 ppb nearby. As can be seen in Figure 3, the model generates a large ozone plume (values > 120 ppb) over Galveston Bay that extends north to near Port Arthur and south to near Freeport TX. Concurrently, the model predicts ozone values from 90-120 ppb into Houston proper (higher in the southern portion of the city). The net effect is that the model underestimates ozone at the highest sites along the shoreline of Galveston Bay, but overestimates ozone at those sites 20-60 miles from the bay. As seen in the statistics above (27% positive bias), the overprediction is very large in the B-PA region.

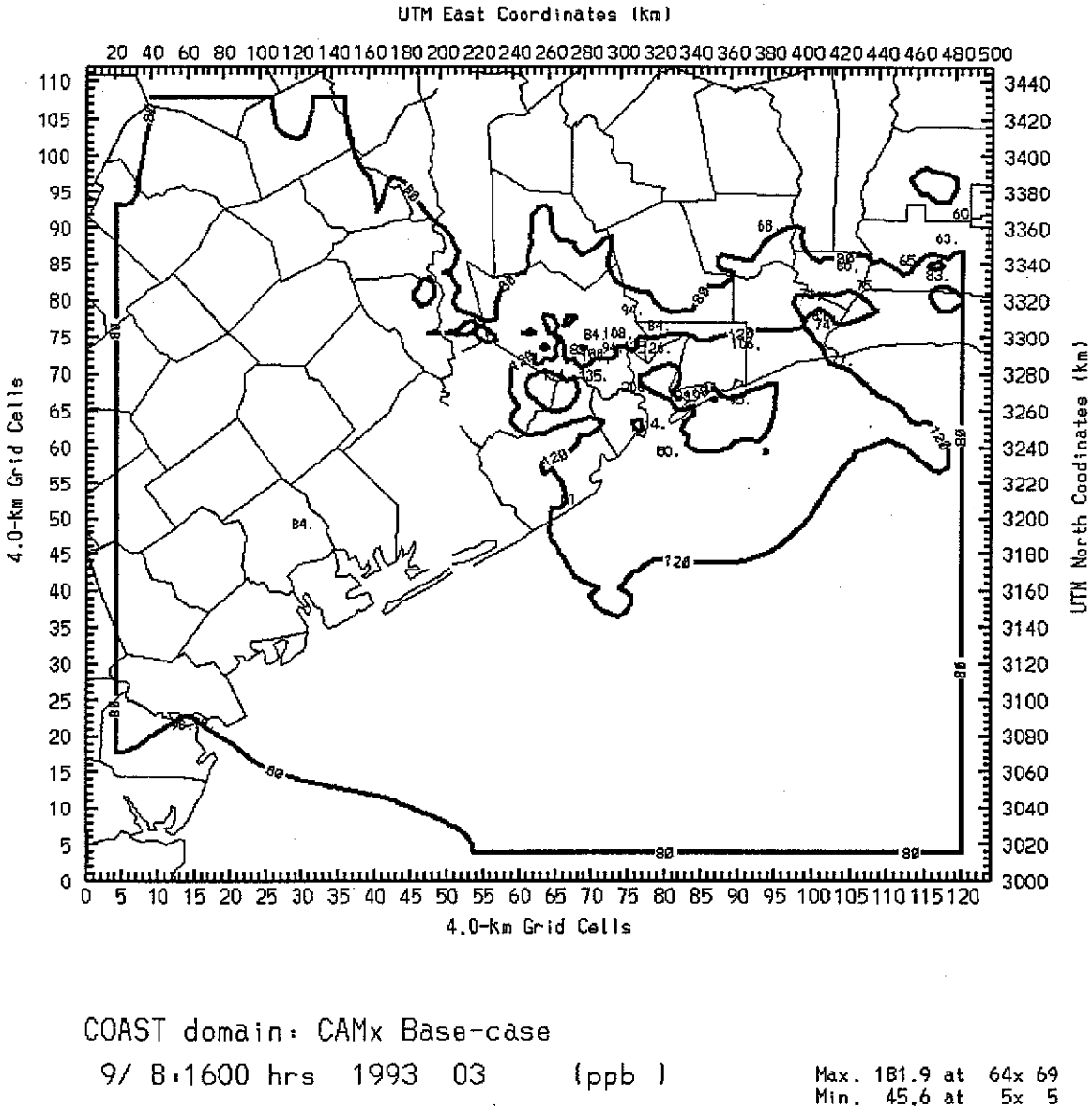

Figure 3. Model ozone isopleth plot with observations overlaid for 4 p.m. CST on 8 September. Contours of 80, 120, and 160 ppb are plotted. Maximum and minimum model predictions for this hour are plotted in the lower right portion of the graph.

Reviewing model ozone animations, it appears that a sea breeze develops around noon on the 8th and is responsible for the model advection of ozone from the Galveston region to the B-PA region. It would be interesting to check the adequacy of the meteorological model in reproducing this particular feature.

On the 9th, peak afternoon ozone values are very high in an extremely localized area over Galveston Bay. Texas City observed 184 ppb of ozone at this hour. Smith Point was in the 150 ppb range. Yet values in Harris County were relatively low (55-85 ppb). The site in Galveston,

while only 98 ppb at 4 pm, had peaked earlier in the day around 125 ppb. The Clute TX site near the Gulf of Mexico was also very high (123 ppb this hour, having peaked around 150 ppb at 3 pm). Meanwhile, the B-PA and Louisiana airsheds were fairly clean (75-90 ppb) and there appeared to be a sharp ozone gradient as one proceeded south in the domain (Victoria ~ 95, Corpus Christi ~ 70). Figure 4 shows the afternoon model and observed ozone fields.

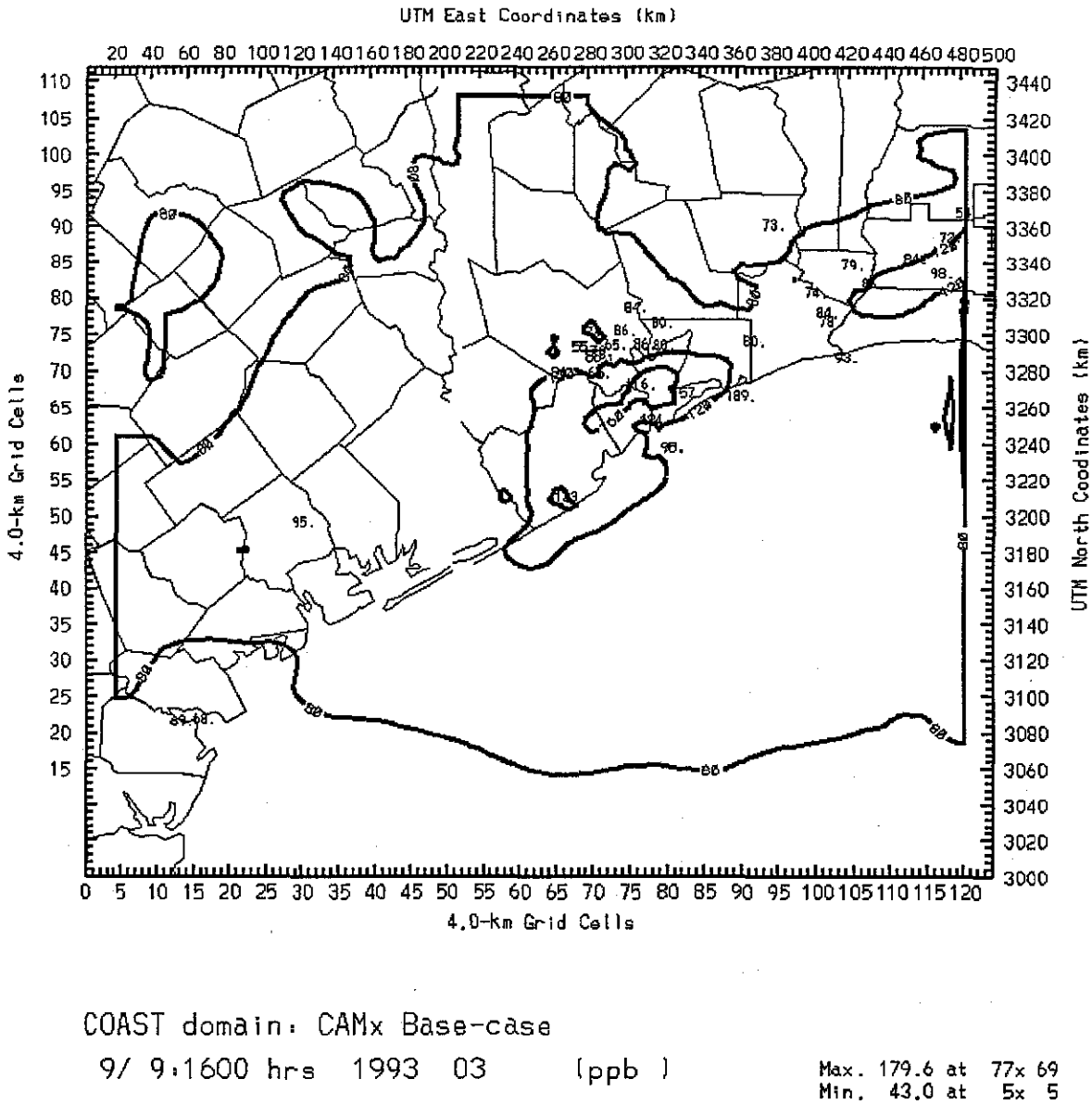

Figure 4. Model ozone isopleth plot with observations overlaid for 4 p.m. CST on September 9th. Contours of 80, 120, and 160 ppb are plotted. Maximum and minimum model predictions for this hour are plotted in the lower right portion of the graph.

From a qualitative standpoint, model performance on the 9th is quite good. The model reproduces the highly localized ozone plume over the mouth of Galveston Bay in space and in magnitude (just slightly too far to the northwest). It also captures the ambient fields in Houston,

B-PA, and the southern cities. There does seem to be a modeling artifact along the eastern boundary on this afternoon that should be investigated.

On September 10th, there is a broad area of elevated ozone (100-140 ppb) ranging from far southeastern Harris through Chambers and into Jefferson county. Observed ozone is relatively low on the other side of the Sabine River in LA and is very low in southern TX.

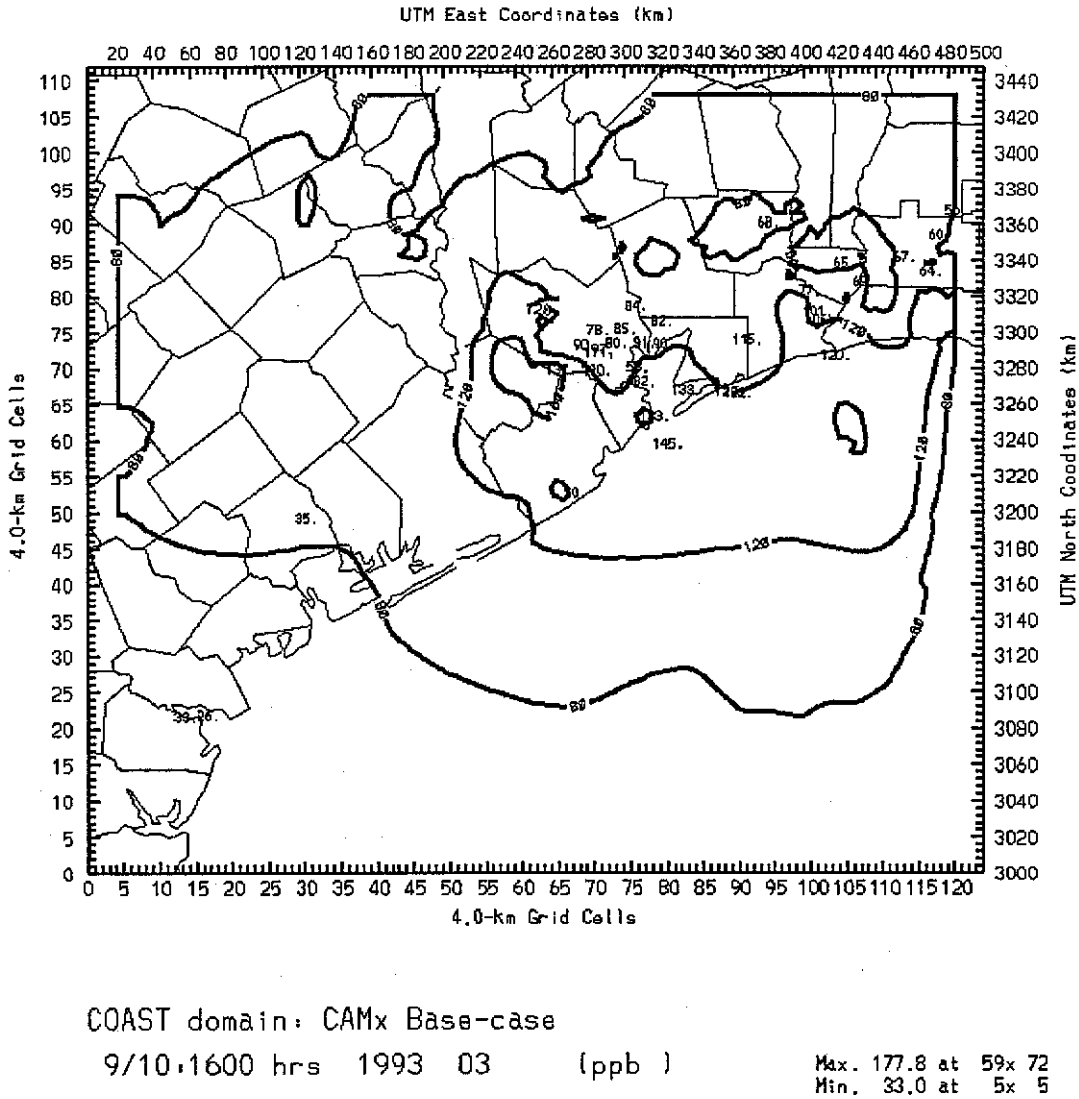

Figure 5. Model ozone isopleth plot with observations overlaid for 4 p.m. CST on September 10th. Contours of 80, 120, and 160 ppb are plotted. Maximum and minimum model predictions for this hour are plotted in the lower right portion of the graph.

At the same time, as seen in Figure 5, model performance is relatively poor. Model ozone is too low in Chambers County and apparently too high in many other locations (Lake Charles, Brazoria County, etc.). The model does capture the clean conditions in Corpus Christi.

By the last day of the episode, air quality is relatively clean by 4 p.m. Most of the elevated ozone on this day occurred in a short burst in the Houston region around noon, as high as 180 ppb. These values appear to have been transported quickly to the north, into an area not covered by the monitoring network, during the afternoon. Figure 6 plots the model and ambient data at noon on the 11th.

The model does not reproduce the short-lived ozone exceedances seen over Houston around noon very well spatially. Even by that hour most of the model ozone (as high as 147 ppb) was in northern Harris County. Furthermore, the unpaired peaks are indicated model underpredictions of 20-40 ppb. Model performance elsewhere during this time period is acceptable.

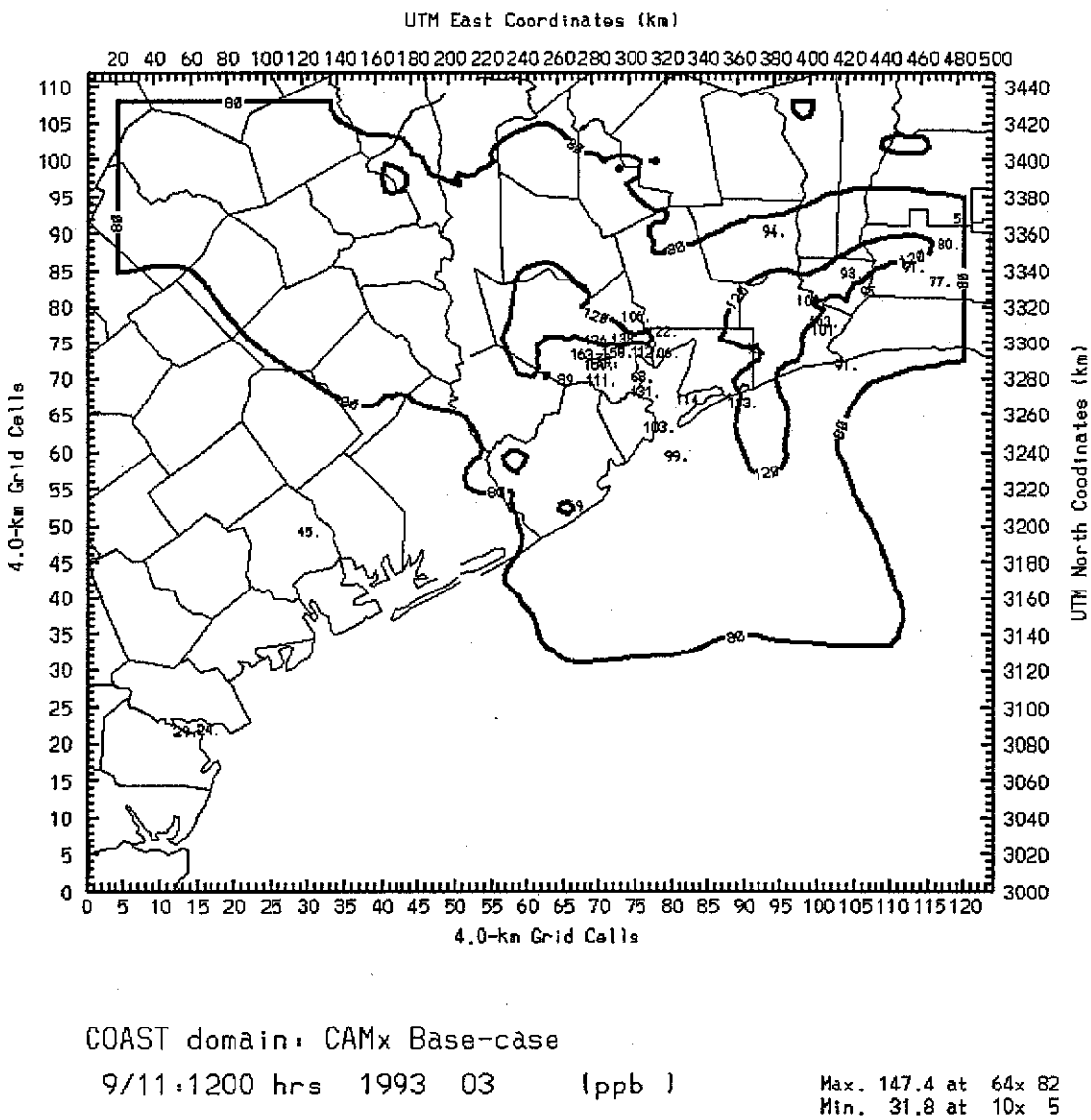

Figure 6. Model ozone isopleth plot with observations overlaid at noon on 11 September. Contours of 80, 120, and 160 ppb are plotted. Maximum and minimum model predictions for this hour are plotted in the lower right portion of the graph.

4. SITE-BY-SITE ASSESSMENT OF MODEL PERFORMANCE

This section will attempt to assess the quality of the H-G base case modeling on a site-by-site basis. As discussed above, assessing model performance statistics can be difficult when comparing a model grid volume average against an observation at a single point in space. The station time series plots analyzed in this section are based on a bilinear interpolation from the four model grid cells surrounding the monitor location. Please remember when viewing these plots that there can be instances when a monitor data point is not representative of an entire grid cell. For the purpose of brevity only a handful of plots will be shown in the body of this document, but model versus observed comparisons can be found for all COAST locations in Appendix C (time series plots) and Appendix D (scatter plots).

4.1 HOUSTON AREA

CLINTON CGC / HARRIS CO TX: The modeling results match the ambient ozone data at this site fairly accurately for the first 3 days of the simulation (see Figure 7a), but performance is relatively poor over the September 9-11. On the 9th, ambient peaks are around 80 ppb whereas the model exceeds 120 ppb in the grid cell. On the 10th, the model is unable to reproduce a late-day ozone buildup (observed ~125, model ~105 ppb). The observed peak of 172 ppb is badly underestimated by the model (~95 ppb). The reason for this underestimation appears to be the strong southerly winds that transport the Houston ozone plume out of Harris County by midday. From the scatter plot shown in Figure 7b, one can see there are a dozen outlier residual pairs, most of these occur late in the afternoon on the 10th.

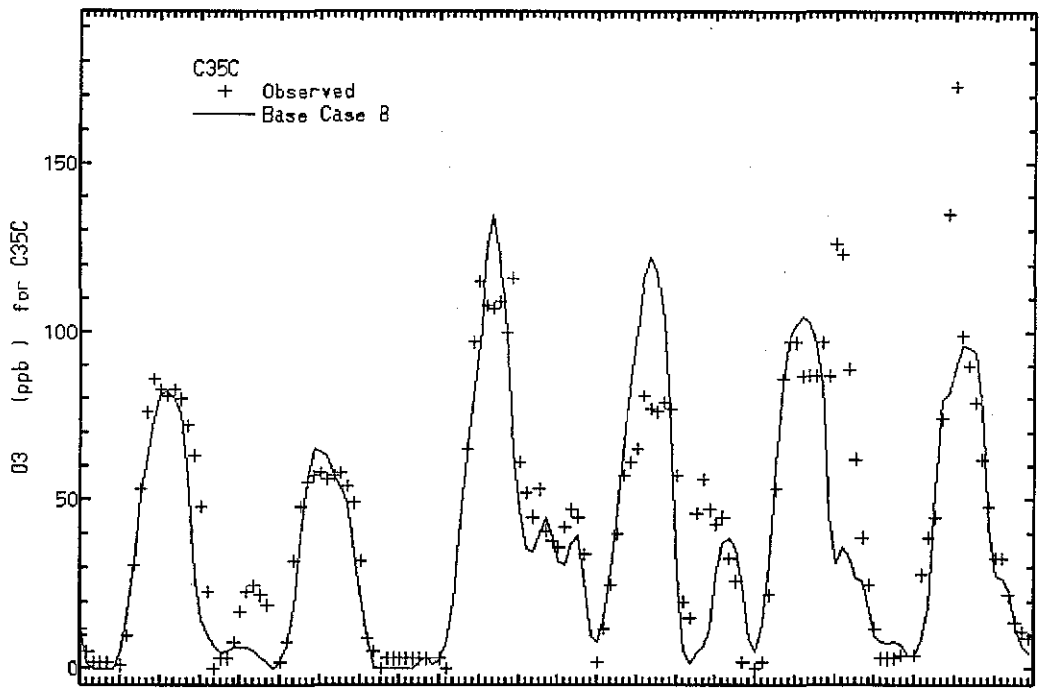

Figure 7a. Time series plot of CAMx base case model ozone and COAST ozone data at the Clinton CGC site (C35C) in Harris county.

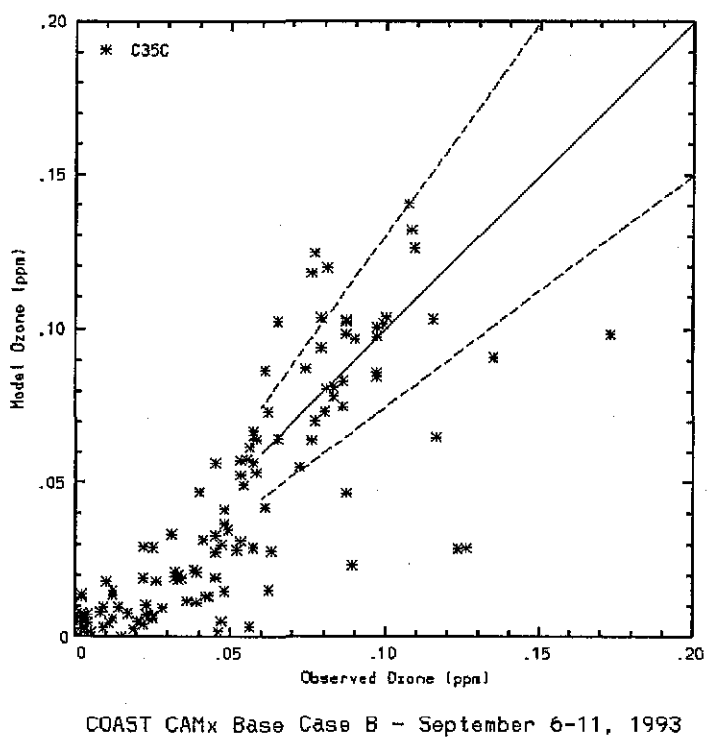

Figure 7b. Scatter plot of CAMx base case model ozone and COAST ozone data at the Clinton CGC site (C35C) in Harris County.

HRM SITE 1 TX: The difference trace (model v. observed) for this monitor is very similar to the Clinton CGC site which is not surprising given their proximity to one another. The model reproduces the ozone peaks with some accuracy on September 6-8, but severely overestimates on the 9th (~40 ppb) and severely underestimates on the 10th-11th (30-90 ppb). As mentioned before, the meteorological fields appear to be responsible for this air quality modeling deficiency.

HRM SITE 3 TX: This Houston site (just to the east of Clinton CGC & HRM Site 1) is generally overestimated in the Base Case. The overpredictions are mild through the first 3 days of the simulation (5-20 ppb), but as at other Houston sites the model predicts approximately 130 ppb on the 9th when the monitor was reading peaks near 80 ppb. Again, on 10 September, the model does not reproduce the late-day ozone buildup, possibly due to insufficient sea breeze penetration, and ozone on the 11th is grossly underestimated (by about 55 ppb).

HRM SITE 4 TX: At this site in northeastern Houston, the model ozone trace is a relatively accurate match of the ambient data trace. On both the 8th and the 10th there is a brief late-day spike in the observed ozone values that is not captured by the model. Like the other Houston sites, ozone is overpredicted around 30-40 ppb on the 9th. The model predictions on September 11 of 120 ppb are close to the observed 140 ppb, which is consistent with the theory discussed in Section 3 that the model plume is being advected too far to the north.

HRM SITE 7 TX: Just east of Houston, the model is performing with relatively little bias. Three noticeable deficiencies: a) the late-day peak on 10th is missed in the model, b) high ambient values on the 11th are underestimated by about 40 ppb, and c) nighttime ozone is generally underestimated.

CROSBY AQ/MET SITE TX: The model reproduces the peak ozone within 0-20 ppb on all days of the episode, except the 8th (where it underpredicts by about 30 ppb). The interesting characteristic of this particular model-observed time series plot is the failure of the model to capture the near-zero ozone at night within this urban grid cell. This is a common feature in photochemical modeling exercises. The key question would be weather this monitoring site truly representative of the entire grid cell or is it affected by sub-grid scale effects (i.e., titration from local NO sources). This site is located in far northeastern part of Harris county.

HRM SITE 8 TX: In the southeastern part of the city, ozone appears to be overestimated by the model. The positive bias was about 10-20 ppb on the 6th and 7th and 30-40 ppb on the 10th and 11th. There was a data gap in the observations on the 8th and 9th that prevented comparisons on those days.

HRM SITE 10 TX: Model performance is excellent at this site near the intersection of Harris, Liberty, and Chambers counties. The peaks are all reproduced within 5-15 ppb and the observed double-humped profiles of the 8th and 10th are reflected in the model time series.

HRM SITE 11 TX: Model performance at this site near Baytown is solid. The model captures both the low ozone on the 6th and 7th (slight overestimations) and the high ozone on the 8th through 11th. The model predicts a double-humped peak on the 9th that is not reflected in the

observations.

SITE T-19 CRAWFORD TX: At this site just to the west of downtown Houston, model performance is similar to other downtown Houston sites (HRM 1, etc.). The first 3 days of the simulation are reasonably reproduced, then the 9th is overestimated and the 10th and 11th are severely underestimated. Interestingly, the model does capture the unusual buildup of ozone on the 9th from 6 P.M. to midnight.

SITE T-18 CROQUET TX: This site is located in far southern Harris county. It is generally characterized by model overpredictions (50 ppb on the 8th, 30 ppb on the 9th and 10th, 40 ppb on the 11th).

MANCHESTER C22 TX: Only sporadic observational data exist, but it appears that the model behavior at this site is very comparable to its neighbors Clinton CGC & HRM #1.

SWISS&MONROE / HARRIS CO TX: This is another far southern Harris county site, but the model vs. observed comparisons here are much better than at Site T-18. Peak daily ozone values are match within 5 ppb on the 6th, 8th, and 11th. Model performance is poor on the 9th with overestimations of 40 ppb.

SITE S-13 N WAYSIDE TX: The last Harris county site to be compared was this northern Houston location. Model performance is poor: peaks are severely overestimated (20-60 ppb) on the first 5 days of the episode, than underestimated on the 11th (observed = ~160; model = ~130 ppb).

4.2 GALVESTON BAY AREA

GALVESTON AS SITE TX: The model overestimates peak surface ozone on the 6th and 8th (by 25-40 ppb), is very accurate on the 7th, 9th, and 11th, and underestimates peak ozone on the 10th (15-20 ppb). One feature seen in this time series and not in the Houston plot is that the model tends to overpredict late evening ozone (6 P.M. to midnight). In other words, the observed ozone drops off much faster than the model ozone. The opposite was found in the Houston comparisons.

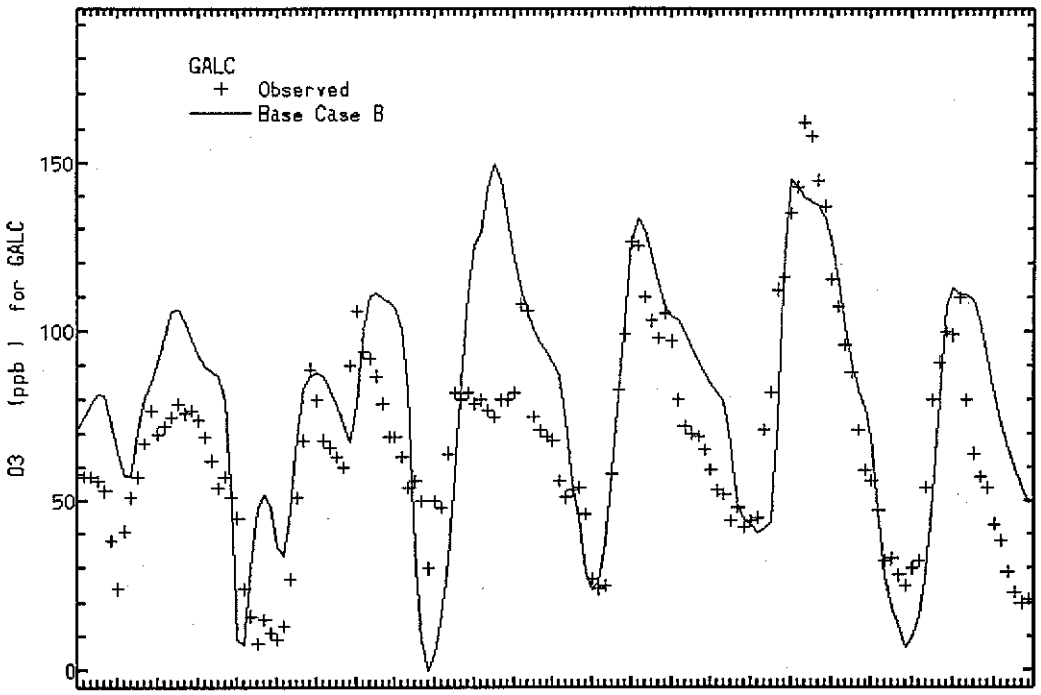

Figure 8a. Time series plot of CAMx base case model ozone and COAST ozone data at the Galveston site (GALC) in Galveston county.

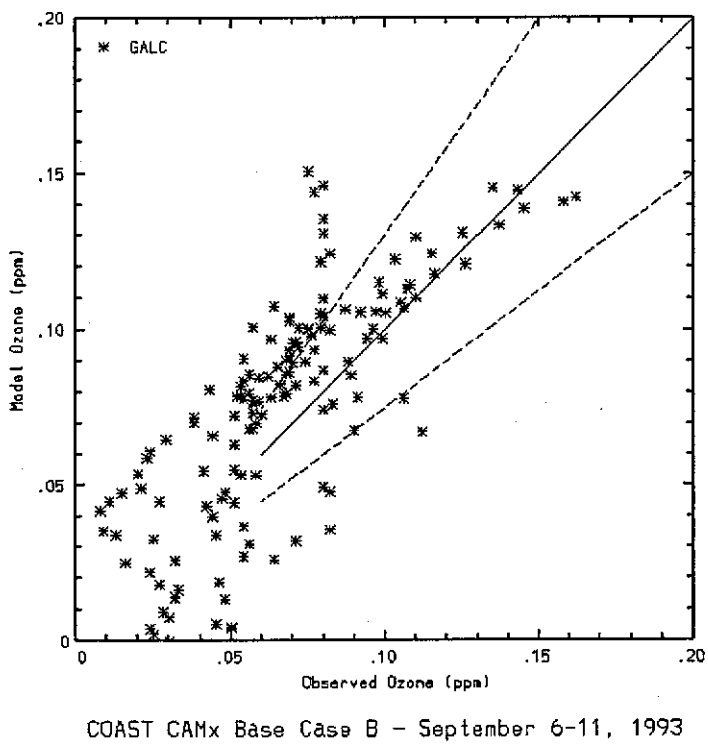

Figure 8b. Scatter plot of CAMx base case model ozone and COAST ozone data at the Galveston site (GALC) in Galveston county.

SEABROOK C20 TX: The Seabrook site is on the western edge of Galveston Bay and is one of the highest ozone sites throughout the episode. Generally, the model performs capably at this location. Underpredictions (20-40 ppb) occur on the 8th and 11th. The 6th, 9th, and 10th, see similar model and observed ozone peaks.

SMITH POINT AQ/MET SITE TX: At this shoreline (Galveston Bay) site, ambient ozone is very high (~180 ppb) on the 8th and 9th, ~150 ppb on the 10th, and ~125 ppb on the 11th. As might be expected at a peak ozone location, the model tends to underestimate ozone, but not drastically so. Model peaks approach 160 ppb on the 8th and 9th, 130 ppb on the 10th, and 115 ppb on the 11th.

STOWELL (WINNIE) AQ/MET TX: This site is located in far northeastern Chambers county. The model captures the peaks within 10-30 ppb (worst overprediction is on the 8th). The most noticeable feature is the overprediction at night.

GILCHRIST TX: There are a couple of modeling deficiencies exhibited by this particular time series comparison. First, there seems to be a 2-4 hour lag in the ozone concentrations. Observed peaks typically occur shortly after midday at this site whereas the model peaks occur around 4 P.M. CST. Second, note the severe underpredictions on the 9th (180 observed, 100 modeled). The model does generate a band of 160-180 ppb ozone near Gilchrist, it has just been advected too far inland. This again points out the severity of a strict monitor to grid cell comparison.

TEXAS CITY / LA MARQUE TX: This site is located on the southwestern edge of Galveston Bay. The model does not reproduce the highest peaks near 180 ppb on the 8th and 9th (model ~ 150 ppb), but does better with the lower peaks on the 10th (~140 ppb) and 11th (~105 ppb).

4.3 BEAUMONT-PORT ARTHUR AREA

BEAUMONT C02/JEFFERSON CO TX: The distinguishing feature of the comparison at this site is the large overpredictions previously explained on 8 September. The model performs reasonably well during the remainder of the episode, with a slight overprediction on the 11th (20-25 ppb).

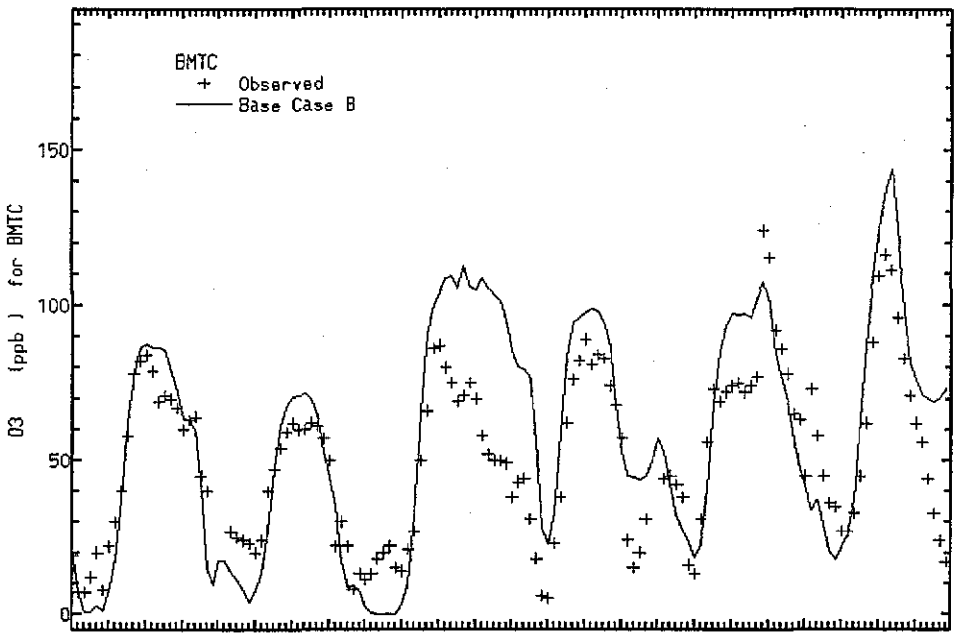

Figure 9a. Time series plot of CAMx base case model ozone and COAST ozone data at the Beaumont site (GALC) in Jefferson county.

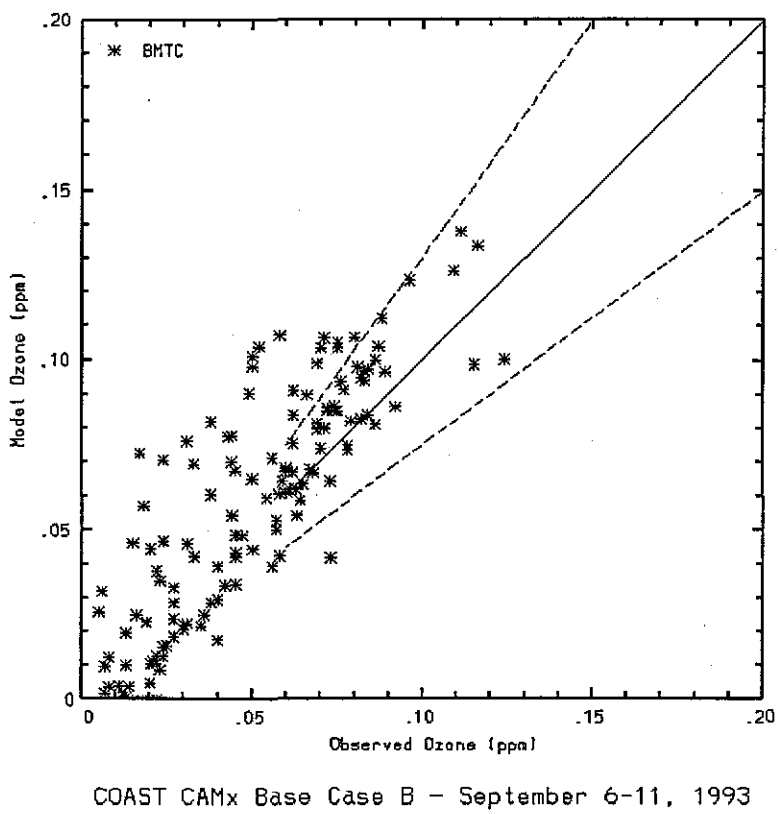

Figure 9b. Scatter plot of CAMx base case model ozone and COAST ozone data at the Beaumont site (BMTC) in Jefferson county.

SETRPC SITE 43 TX: At this site in Port Arthur, the model overpredicts observed ozone for the first three days of the episode by about 10-20 ppb. The model is quite accurate in estimating daily peak ozone over the remaining three days, however. The ozone does not fall off as sharply at night in the model as is seen in the observations.

PORT ARTHUR WEST C28 TX: Model performance at this site is similar to the other Port Arthur site. Mild overpredictions occur early in the episode, but exceptional model performance is exhibited on the 9th-11th.

SETRPC SITE 40 TX: At this site located near Sabine Pass TX along the Gulf of Mexico shoreline, ozone is strongly overestimated (observed ~ 80; model ~ 130) on 8 September. The remainder of the episode features accurate model performance with a slight tendency for model ozone to stay higher longer into the evening than observed.

SETRPC SITE 42 TX: This monitor is located in central Orange county. The most noticeable feature is the failure of the model to reproduce the ozone decrease overnight on the 8th-9th. While the observations drop down to zero, the ozone concentrations remain about 100 ppb in the model. As discussed above, this results from the transport of Gulf of Mexico ozone into this region during this period. In general, this site is marked by an positive model bias.

KOUNTZE C85/HARDIN CO TX: The Kountze monitor is located in a rural region about 40 km north of Beaumont. Ozone is generally low at this site, exceeding 100 ppb only on September 11th. The model tends to overestimate the peaks in this region, especially on the 8th and 11th. Also, the model does not reproduce the presumably local titration effects at night.

CAMS 9, West Orange, TX: Model behavior is similar at this Orange county site as in the SETRPC SITE 42. Note the positive model bias on the 9th. Interestingly, this is the lone B-PA site that performs satisfactorily on 8 September.

4.4 SOUTHWEST LOUISIANA SITES

Vinton-Calcasieu; Westlake-Calcasieu; Carlyss-Calcasieu; Ragley-Beauregard: In general, the model tends to exhibit a positive bias at these 4 Louisiana locations. The worst time series comparisons are for the Carlyss monitor that is usually affected by an apparently exaggerated Lake Charles plume in the modeling. The Vinton site exhibits relatively little bias.

4.5 BACKGROUND AREAS

CLUTE CAMS 11/BRAZORIA CO TX: The model does not reproduce the magnitude of the peaks on the 7th and 9th at this Brazoria county site located relatively close to the Gulf of Mexico shoreline. This comparison is also one of the few where the model tends to be too low at night relative to the observations.

VICTORIA REGIONAL (CAMS) TX: Negative aspects of model performance include: 1) trouble with diurnal ozone profiles early in episode and 2) the low ozone on the last 2 days of the episode is overestimated. Positive aspects of model performance are: 1) magnitude of peaks on 8th and 9th match observations closely, and 2) model does reproduce general cleansing of air quality late in the episode.

WEST C4 TX and TULOSA C21 TX: For both of these sites in the Corpus Christi area, the model reproduces the key days (i.e., high ozone days) of the 8th and 9th with some precision. Overpredictions are common on the early and later portions of the episode, although the general episode air quality trend is modeled with a fair amount of skill.

5. DIAGNOSTIC EVALUATION AND TESTING

Diagnostic tests are designed to check the model formulation and the response to various inputs. Given an unlikely extreme input condition (e.g., zero emissions), the model results are checked to determine that the model produces an appropriate response. Generally, a series of tests are run on the emissions, meteorological inputs, and boundary conditions. Four diagnostic simulations were performed for the H/G area, as follows:

- zero all emissions (anthropogenic and biogenic)
- zero boundary and initial conditions
- reduce wind speeds by 50 percent
- reduce biogenic VOC emissions estimates by 50 percent

The goal of diagnostic testing is to determine whether the model exhibits expected behavior under extreme changes to its input. Diagnostic tests check for spurious behavior that might indicate problems in the model formulation. Overall the results of the four CAM_X diagnostic tests were consistent with expectation.

5.1 EFFECT OF ZERO EMISSIONS INVENTORY

Zeroing out emissions from the CAMx modeling has the following effects:

- Daily peak ozone values over the Texas domain are sharply reduced (40-120 ppb). After the first 24 hours, the only concentrations greater than 60 ppb in the domain were attributable to inflow from the eastern or northern boundaries.

- In some urban areas, there were some ozone increases on the order of 10-40 ppb at night without emissions. On 7 September, where NO titration kept ozone in a few Houston grid cells near zero, there were some small ozone increases.

- The response of the model was exactly what was expected. This particular diagnostic test did not reveal any flaws in the CAMx model formulation.

Figure 10 shows a comparison of the base case and zero emissions simulations at the hour of peak ozone on 9 September 1993. One can see the two urban plumes no longer exist downwind of H-G and BPA once emissions are zeroed

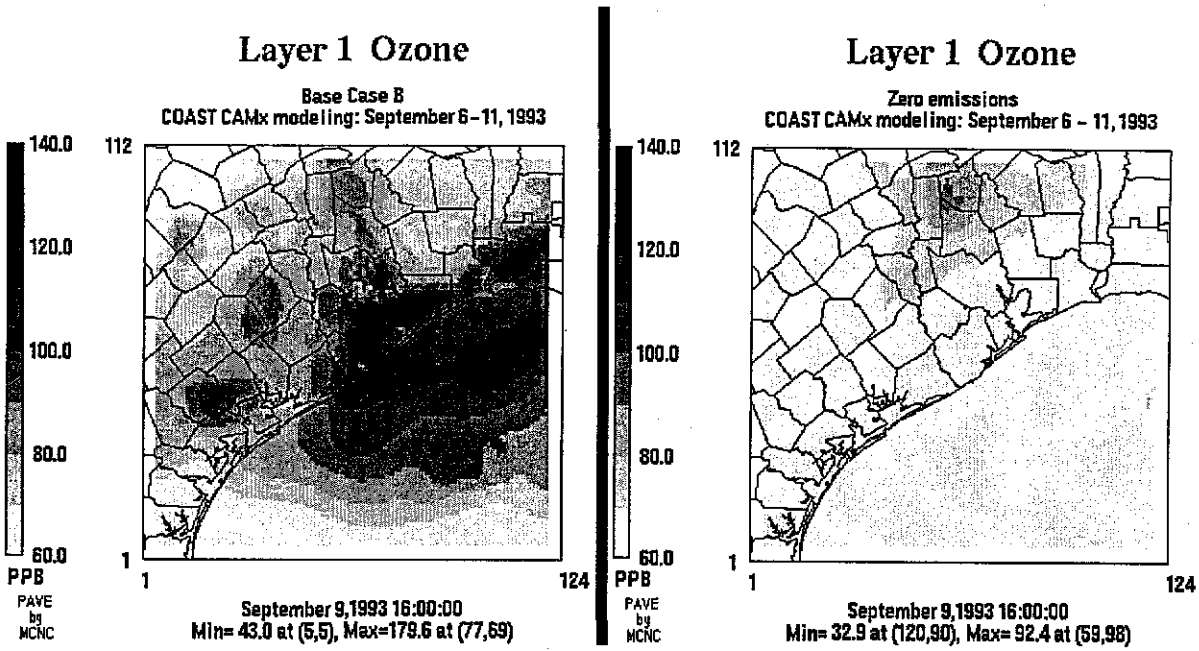

Figure 10. Simulated ozone concentrations for 1600 CST, 9 September 1993. Left side of plots is for the base case simulation. Right side of the plots is for the simulation with zero emissions.

5.2 EFFECT OF ALTERNATE BASE YEAR EMISSIONS INVENTORY

Reducing biogenic VOC emissions by 50% in the COAST CAMx modeling has the following effects:

- Daily peak ozone values over the domain are reduced (15-40 ppb).

- There is a regional ozone response as domainwide ozone is reduced by about 5-10 ppb on average. The majority of the model response took place downwind of urban NOx plumes.
- The response of the model was exactly what was expected. In fact, the results were quite similar to a prior sensitivity run in which urban biogenic emissions were reduced. Figure 11 shows the model ozone response at a typical afternoon hour.

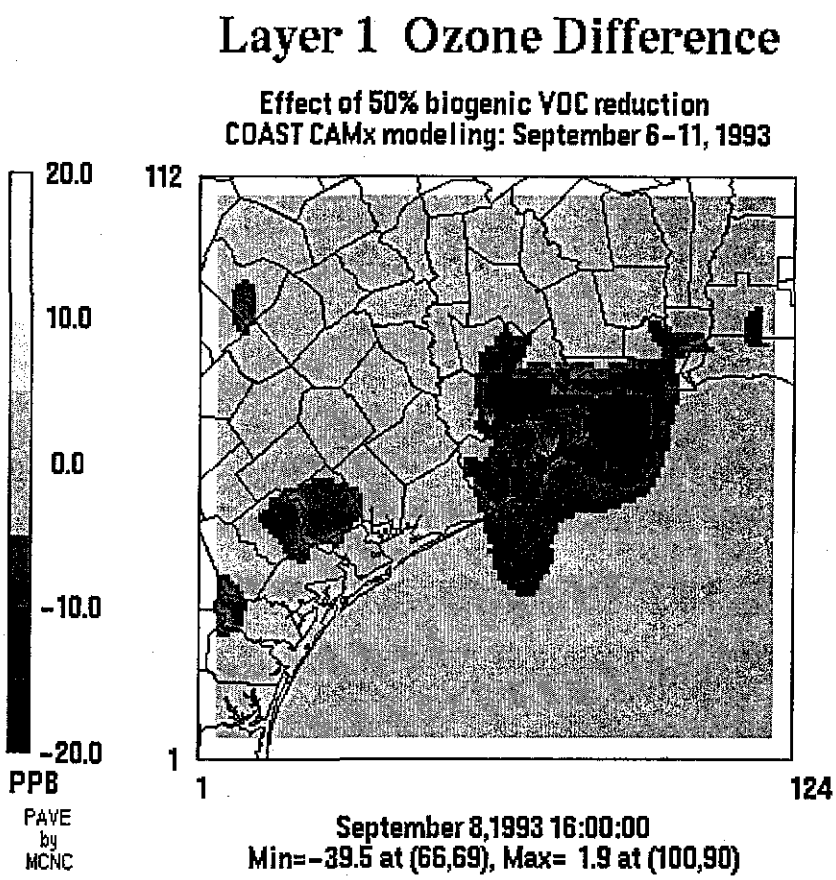

Figure 11. Simulated ozone reductions in response to a 50 percent cut in biogenic VOC emissions at 1600 CST on 8 September 1993.

5.3 EFFECT OF ZERO INITIAL AND BOUNDARY CONDITIONS

Zeroing out initial and boundary conditions from the CAMx modeling has the following effects:

- Daily peak ozone values over the Texas domain are sharply reduced (40-120 ppb) on the initial day of the simulation and slightly less on 7 September.

- Generally, model ozone concentrations were lower (10-50 ppb) in the scenario without initial condition carryover or boundary condition transport.

- The response of the model was exactly what was expected. This particular diagnostic test did not reveal any flaws in the CAMx model formulation. Figure 12 shows the simulated ozone concentrations with and without initial and boundary conditions.

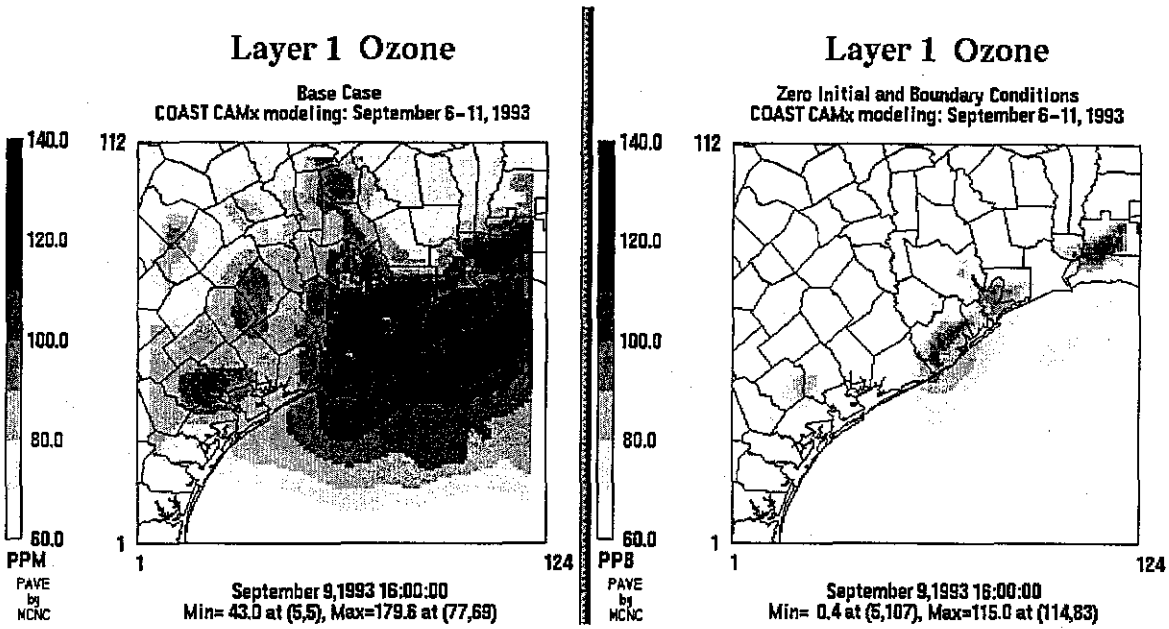

Figure 12. Ozone concentration fields at 1600 CST on 9 September 1993. The left half of the plots are the base case fields and the right half are the simulations with zero initial and boundary conditions.

5.4 EFFECT OF REDUCED BASE YEAR WIND SPEEDS

The final simulation completed during this part of the exercise looked at the sensitivity of the model to reducing wind speeds by 50 percent. Figure 13 shows the resultant effect on the simulated ozone concentrations.

Reducing the input wind speeds by a factor of two over the COAST CAMx modeling has the following effects:

- Daily peak ozone values over the Texas domain are increased (20-100 ppb).
- Simulated ozone was increased domainwide, especially close to the urban areas.
- The only areas to exhibit ozone decreases with the new wind field were those locations affected by urban ozone plumes late in the day.
- From a model performance standpoint, model bias would be prohibitive with this particular wind field.
- It is concluded that the model base year simulations are highly sensitive to wind magnitudes.

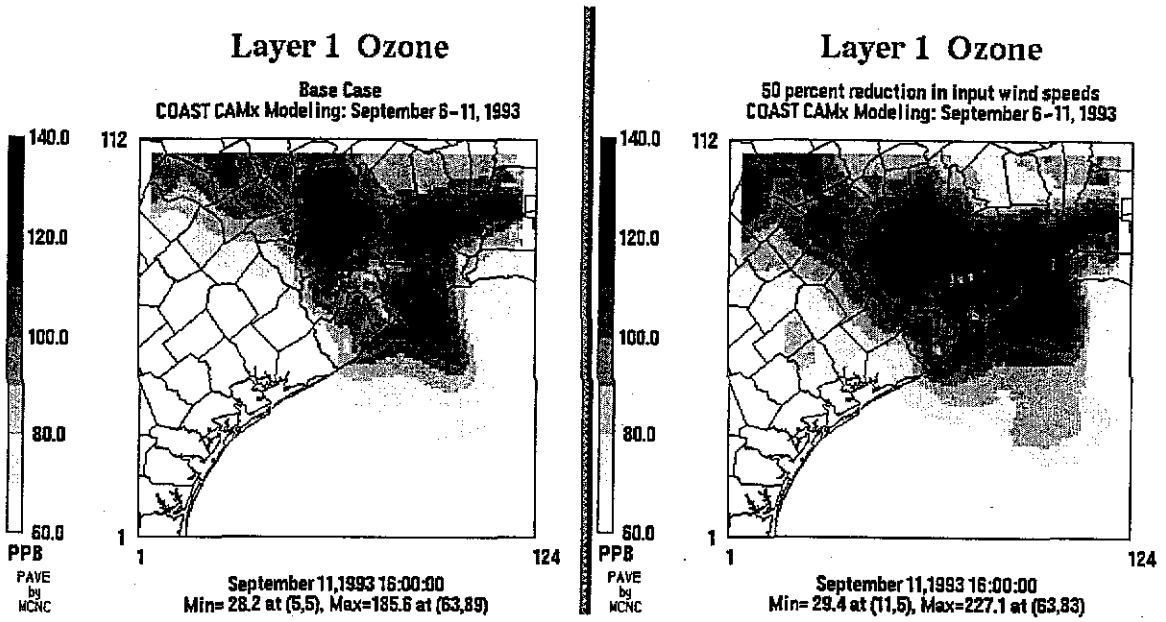

Figure 13. Simulated ozone concentrations for 1600 CST, 11 September 1993. Left side of plots is for the base case simulation. Right side of the plots is for the simulation with wind speeds reduced by 50 percent.

6. CONCLUSIONS AND RECOMMENDATIONS:

In general, CAM_X **model performance is acceptable** for the September 1993 COAST episode. This is based primarily on the statistical analyses presented in Section 2 of this report, in addition to the qualitative (Section 3) and site-by-site (Section 4) assessments. Additionally, the results from the diagnostic testing bolster the acceptability of the modeling exercise. While the model appears to be sufficient for use as technical support to guide air quality planning issues, there are a few modeling features that should be recognized as this work proceeds.

- There is generally a positive bias (overprediction) in the base year CAM_X results.
- The period and region of poorest model performance is on 8 September in the Beaumont-Port Arthur region. It appears as if the input wind fields result in excessive transport of offshore ozone into the region.
- The model underestimates ozone observations in the 120-180 ppb range and overestimates ozone in the 60-80 ppb range.
- Model performance statistics also indicate acceptable model performance when considered on a subregional basis, with the exception of B-PA on the 8th.
- None of the diagnostic/sensitivity tests indicated any major problems with the CAM_X

model formulation. In general, the model performed as expected, as a function of prescribed input changes.

In terms of possible model improvements, additional evaluation and revision of the meteorological fields would likely yield the greatest improvements to CAM_X model performance. Previous meteorological evaluations have uncovered errors and biases in the original COAST meteorological modeling (TNRCC, 1998a). As seen in the evaluation analyses discussed above, deficiencies in the input wind fields can have a large impact on the accuracy of the air quality predictions. In particular, the thermal flows (land breeze/ sea breeze) along Galveston Bay and the Gulf of Mexico should be closely scrutinized.

Also, an additional element of uncertainty in a photochemical modeling exercise, such as this, is the emissions estimates. TNRCC has devoted considerable effort to developing an accurate emissions inventory. Sensitivity runs performed throughout the course of the study based on inventory revisions have shown that simulated ozone is highly sensitive to changes in urban emissions in particular (MCNC, 1999b). It is recommended that effort be made to "evaluate" the inventory estimates by reconciling them against ambient data whenever possible. Analyses such as these, in combination with a successful model performance evaluation, further bolster the confidence one has in using a model to guide air quality attainment planning.

7. REFERENCES

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Texas Natural Resource Conservation Commission, 1998: *Protocol for Ozone Modeling of the Houston-Galveston area with the Comprehensive Air Quality Model with Extensions (CAMx) and COAST Data.* Austin, TX.

Due to the length, the appendices associated with this report
are not available in electronic file.

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TCEQ to attain a hardcopy version.