Appendix D

Report - Migration of the Beaumont/Port Arthur Ozone Modeling from UAM-V to CAMx

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Migration of the Beaumont - Port Arthur Ozone Modeling from UAM-V to CAM_X

Prepared for:

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1. INTRODUCTION

The ultimate goal of the Beaumont-Port Arthur (B-PA) modeling study is to evaluate the effectiveness of candidate control strategies in demonstrating attainment of the one-hour National Ambient Air Quality Standard (NAAQS) for ozone in the three-county B-PA ozone nonattainment area. An initial step in this process to is link past modeling simulations done for the airshed with analyses using a newer, publicly available, photochemical grid model. This report summarizes the differences in simulated air quality between the Urban Airshed Model (UAM) and the Comprehensive Air Quality Model with Extensions (CAMx) for the 31 August – 2 September COAST episode.

In order for air quality models to be successfully used as technical support for a regulatory initiative they must be physically sound. Furthermore, in a regulatory environment it is crucial that oversight groups (e.g., the Environmental Protection Agency), the regulated community, and the interested public also be convinced of the suitability of the model. The model performance evaluation described in the B-PA modeling protocol (Texas Natural Resource Conservation Commission, 1998) is designed to demonstrate that the model is a valid tool for the identification of potential emissions control strategies.

Additionally, to ensure that a modeling study is defensible, the model must be scientifically appropriate for the intended application and the source code must be freely accessible to all stakeholders. Adhering to this principle encourages contributive peer review and allows those to be affected by the eventual control strategies to reproduce the modeling and to test possible alternate strategies that were not simulated as part of the regulatory process.

The preliminary stages of the B-PA modeling used the Variable-Grid Urban Airshed Model (UAM-V) (SAI, 1996). However, because the UAM-V model was not available on a timely basis and at a reasonable cost to outside parties, the Texas Natural Resource Conservation Commission (TNRCC) determined that the publicly available CAM_X model (Environ, 1997) was a more suitable platform to perform the photochemical modeling simulations. Like UAM-V, CAM_X is based on well-established treatments of advection, diffusion, deposition, and chemistry.

In this portion of the B-PA modeling study we ran the CAMX model using the same set of inputs previously used in UAM-V and compared the model outputs over the B-PA domain for the August 31st to September 2nd 1993 COAST base year episode. Descriptions of the spatial and temporal differences between the two sets of results for ozone and key precursors are provided, as well as possible explanations for these differences. The purpose of these comparisons is to ensure that the B-PA modeling results do not vary greatly between these two models, thereby guaranteeing the continued relevance of the previous B-PA modeling analyses.

2. ACQUISITION OF DATA FILES

The first step in the process of comparing the existing UAM-V model results to CAM_X model results for the B-PA domain was to acquire the needed CAM_X/UAM-V input and UAM-V output. Three separate data sets were acquired from the TNRCC anonymous file transfer protocol (FTP) server: *ftp.tnrcc.state.tx.us*. Table 2-1 lists the UAM-V input files used in the CAM_X/UAM-V comparisons. Table 2-2 is a listing of the UAM-V output files generated by TNRCC. Finally, Table 2-3 lists the pollutant observation files acquired from the TNRCC FTP server.

It should be noted that it was necessary to reformat the observational data to match CAM_X postprocessing formats. These files are available upon request. Also, CAM_X requires a fine-grid height-pressure file that was not available from the previously completed UAM-V modeling. MCNC created the needed file based on the coarse-grid data.

Table 2-1. UAM-V/CAM_X Input Files

FTP Server Directory:
/pub/AirQuality/AirQualityPlanningAssessment/Modeling/COAST/UAMV_input

Initial Conditions:	uamv_ic.930831.uamv124_reg	
Boundary Conditions:	uamv_bc.930831.uamv124_reg	
	uamv_bc.930901.uamv124_reg	
	uamv_bc.930902.uamv124_reg	
Top Concentrations:	uamv_tc.clean	
Albedo/Haze/O_3 Col:	uamv_aho.930831-930902.coast_16km+hgbpa_04km	
Land Use Type:	uamv_landuse.coast_16km.gz	
	uamv_landuse.hgbpa_04km.gz	
Photolysis Rates:	uamv_photorate.930831-930902.isop	
Emissions:	uamv_el_ei.930831.93.base.regular	(Elevated pt. source)
	uamv_el_ei.930901.93.base.regular	
	uamv_el_ei.930902.93.base.regular	
	uamv_lo_ei.930831.coast_16km.93.base.regular	(Low area source)
	uamv_lo_ei.930831.hgbpa_04km.93.base.regular	
	uamv_lo_ei.930901.coast_16km.93.base.regular	
	uamv_lo_ei.930901.hgbpa_04km.93.base.regular	
	uamv_lo_ei.930902.coast_16km.93.base.regular	

uamv_lo_ei.930902.hgbpa_04km.93.base.regular

Table 2-2. Model Output files provided by TNRCC

FTP Server Directory:
/pub/AirQuality/AirQualityPlanningAssessment/Modeling/COAST/UAMV_output

uamv_avrg.930831.93.base.regular.coast_16km
uamv_avrg.930831.93.base.regular.fg
uamv_avrg.930901.93.base.regular.coast_16km
uamv_avrg.930901.93.base.regular.fg
uamv_avrg.930902.93.base.regular.coast_16km
uamv_avrg.930902.93.base.regular.fg

Table 2-3. Pollutant Observation files provided by TNRCC

FTP Server Directory: /pub/AirQuality/AirQualityPlanningAssessment/Modeling/file_transfer

O3.coast.dat
CO.coast.dat
FORM.coast.dat
HCHO.coast.dat
ISOP.coast.dat
NO.coast.dat
NO2.coast.dat
NOX.coast.dat

3. CAMX SIMULATIONS

The simulation script used to model the B-PA base year run in CAMx is provided in Table 3.1. CAMx version 1.13 (dated January 1998) code was used in the simulations as downloaded from the CAMx web page. During the course of the project, MCNC was made aware of some minor model code changes that were not part of the downloadable CAMx version 1.13. A comparison of a TNRCC run which incorporated the changes and an MCNC run with the original code for a separate episode showed negligible differences.

Since the completion of this run, an updated version of the CAMx model (version 2.00) has been released (Environ, 1998). Should TNRCC decide to switch to the updated CAMx, some comparisons back to Version 1.13 may be warranted.

Table 3.1 Beaumont-Port Arthur CAMx base year simulation script

```
set verbose
#
set INCHEMP  = "/tmp/pdolwick/tnrcc"
set INCOMMON = "/tmp/pdolwick/tnrcc/common"
set INEI     = "/tmp/pdolwick/tnrcc/ei"
set INMET    = "/tmp/pdolwick/tnrcc/met"
set INICBC   = "/tmp/pdolwick/tnrcc/bc-ic-tc"
set OUTPUT   = "/tmp/pdolwick/tnrcc/output"
set HOME     = "/home/com/pdolwick/tnrcc/camx/run"
#
date
#
#   Script to Run CAMx
#
#  --- Create the day 1 input file (always called CAMx.in)
#
cat << ieof > CAMx.in
CAMx COAST Base Case: one HG/BPA 4x4km subgrid, 930831  (MCNC vsn)
Root output name    |$OUTPUT/camx.930831.base_camx113
Start time/date     |   0. 930831
End time/date       |2400. 930831
DT:max,in,emis,out  |0.5 1. 1. 1.
nx,ny,nz            |31  28  8
xorg,yorg,dx,dy     |4. 3000.  16.  16.
time zone,UTM zone  |6 15
PiG parameters      |2000. 12.
Avg output species  |23
                    |NO        NO2       O3        OLE       PAN       NXOY
                    |PAR       TOL       XYL       FORM      ALD2      ETH
                    |CRES      MGLY      OPEN      PNA       CO        HONO
                    |H2O2      HNO3      ISOP      MEOH      ETOH
Num fine nest       |1
i1,i2,j1,j2,nz,mesh |11 30 11 25 8 4
Restart             |false
Chemistry           |true
Dry dep             |true
Wet dep             |false
PiG submodel        |true
UTM cartesian grid  |true
Staggered winds     |false
```

```
Treat area emiss    |true
Treat point emiss   |true
1-day emiss inputs  |false
3-D average file    |true
Source Apportion    |false
Chemparam           |$INCHEMP/CAMx.chemparm.3
Photolysis rates    |$INCOMMON/uamv_photorate.930831-930902.isop
Landuse             |$INCOMMON/uamv_landuse.coast_16km
Height/pressure     |$INMET/uamv_zp.930831.coast_16km
Wind                |$INMET/uamv_wind.930831.coast_16km
Temperature         |$INMET/uamv_temp.930831.coast_16km
Water vapor         |$INMET/uamv_hum.930831.coast_16km
Cloud cover         |
Rainfall            |
Vertical diffsvty   |$INMET/uamv_kv.930831.coast_16km
Initial conditions  |$INICBC/uamv_ic.930831.uamv124_reg
Boundary conditions|$INICBC/uamv_bc.930831.uamv124_reg
Top concentration   |$INICBC/uamv_tc.clean
Albedo/haze/ozone   |$INCOMMON/uamv_aho.930831-930902.coast_16km+hgbpa_04km
Point emiss         |$INEI/uamv_el_ei.930831.93.base.regular
Area emiss          |$INEI/uamv_lo_ei.930831.coast_16km.93.base.regular
Landuse         #1  |$INCOMMON/uamv_landuse.hgbpa_04km
Height/pressure #1  |$INMET/uamv_zp.930831.hgbpa_04km
Wind            #1  |$INMET/uamv_wind.930831.hgbpa_04km
Vertical diff   #1  |$INMET/uamv_kv.930831.hgbpa_04km
Area emiss      #1  |$INEI/uamv_lo_ei.930831.hgbpa_04km.93.base.regular
Coarse grid restart|
Fine grid restart   |
PiG restart         |
ieof
#
#  --- Execute the model ---
#
/bin/time /home/com/pdolwick/tnrcc/camx/bin/CAMx1.13  |& tee
camx.930906.base_camx113.out
date
foreach today (01 02)
set yesterday = `echo $today | awk '{printf("%2.2d",$1-1)}'`
set todate = `echo $today   awk '{printf("%2.2djul95",$1)}'`
date
#   -
#   Script to Run CAMx
#
#  --- Create the input file (always called CAMx.in)
#
cat << ieof > CAMx.in
CAMx COAST Base Case: one HG/BPA 4x4km subgrid, 9309$today  (MCNC vsn)
Root output name    |$OUTPUT/camx.9309$today.base_camx113
Start time/date     |   0. 9309$today
End time/date       |2400. 9309$today
DT:max,in,emis,out  |0.5 1. 1. 1.
nx,ny,nz            |31  28  8
xorg,yorg,dx,dy     |4. 3000.  16.  16.
time zone,UTM zone  |6 15
PiG parameters      |2000. 12.
Avg output species  |23
                    |NO        NO2       O3        OLE       PAN       NXOY
                    |PAR       TOL       XYL       FORM      ALD2      ETH
                    |CRES      MGLY      OPEN      PNA       CO        HONO
                    |H2O2      HNO3      ISOP      MEOH      ETOH
Num fine nest       |1
i1,i2,j1,j2,nz,mesh|11 30 11 25 8 4
Restart             |true
```

```
Chemistry            |true
Dry dep              |true
Wet dep              |false
PiG submodel         |true
UTM cartesian grid   |true
Staggered winds      |false
Treat area emiss     |true
Treat point emiss    |true
1-day emiss inputs   |false
3-D average file     |true
Source Apportion     |false
Chemparam            |$INCHEMP/CAMx.chemparm.3
Photolysis rates     |$INCOMMON/uamv_photorate.930831-930902.isop
Landuse              |$INCOMMON/uamv_landuse.coast_16km
Height/pressure      |$INMET/uamv_zp.9309$today.coast_16km
Wind                 |$INMET/uamv_wind.9309$today.coast_16km
Temperature          |$INMET/uamv_temp.9309$today.coast_16km
Water vapor          |$INMET/uamv_hum.9309$today.coast_16km
Cloud cover          |
Rainfall             |
Vertical diffsvty    |$INMET/uamv_kv.9309$today.coast_16km
Initial conditions   |
Boundary conditions  |$INICBC/uamv_bc.9309$today.uamv124_reg
Top concentration    |$INICBC/uamv_tc.clean
Albedo/haze/ozone    |$INCOMMON/uamv_aho.930831-930902.coast_16km+hgbpa_04km
Point emiss          |$INEI/uamv_el_ei.9309$today.93.base.regular
Area emiss           |$INEI/uamv_lo_ei.9309$today.coast_16km.93.base.regular
Landuse          #1  |$INCOMMON/uamv_landuse.hgbpa_04km
Height/pressure  #1  |$INMET/uamv_zp.9309$today.hgbpa_04km
Wind             #1  |$INMET/uamv_wind.9309$today.hgbpa_04km
Vertical diff    #1  |$INMET/uamv_kv.9309$today.hgbpa_04km
Area emiss       #1  |$INEI/uamv_lo_ei.9309$today.hgbpa_04km.93.base.regular
Coarse grid restart|$OUTPUT/camx.9309$yesterday.base_camx113.inst.2
Fine grid restart  |$OUTPUT/camx.9309$yesterday.base_camx113.finst.2
PiG restart        |$OUTPUT/camx.9309$yesterday.base_camx113.pig
ieof
#
#  --- Execute the model ---
#
/bin/time /home/com/pdolwick/tnrcc/camx/bin/CAMx1.13  |& tee
camx.9309$today.base_camx113.out
date
end
```

4. CAMX AND UAM-V COMPARISON

The remainder of this report presents the results from the comparison of the previous UAM-V base year simulation with the CAMx base year simulation for the August 31st -- September 2nd COAST episode. In a comparison of OTAG modeling data sets, Kumar and Lurmann (1997) found only minor variance between the two predicted ozone fields in terms of model performance quality. This was consistent with a parallel comparison of the two models for the July 1995 Ozone Transport Assessment Group (OTAG) modeling (Jang, 1998).

In a companion report done for the 1993 Houston-Galveston COAST episode (September 6-11th), MCNC (1999) determined that ozone concentrations were consistently 4-9 ppb higher in the CAM_X simulations than in UAM-V. Several possible reasons for the differences between the two models were noted, including: varying treatment of subgrid point source plumes, contrasts in the means by which mass is transferred between the coarse and fine grids, and modifications to the chemical solver. However, MCNC (1999) also concluded that general model performance for surface ozone was similar in UAM-V and CAM_X.

Several simple analyses were performed to assess the similarity of the two model simulations over the B-PA domain. First, pollutant difference animations (CAM_X - UAM-V) were prepared for the period using MCNC's PAVE software. The resultant MPEG files were placed on a private web site for TNRCC review and subsequently released to the Technical Oversight Committee (*http://envpro.ncsc.org/projects/TNRCC-TOC*). Second, time series plots were prepared comparing observed air quality to the surface-level concentrations generated by the two models. These analysis products were generated for the following pollutants: ozone, carbon monoxide, nitric oxide, nitrogen dioxide and volatile organic compounds. Third, isopleth plots of surface ozone in CAM_X and UAM-V, along with plots of ozone differences between the two models were prepared.

4.1 TIME SERIES ANALYSES

In general, average simulated afternoon ozone is 3-7 ppb higher in the CAM_X modeling than in the UAM-V model runs using the same input files (see Figure 4-1). As can be seen in the figure, the differences are greatest during the period in which ozone values are highest (i.e., 3-6 p.m. local time). At night the models maintain comparable amounts of ozone at the surface. The diurnal pattern of the differences is very similar on the 1st and 2nd and also compares very closely to the patterns seen in the Houston-Galveston comparison. Interestingly, the CAM_X to UAM-V differences are slightly smaller for this episode (3-7 ppb instead of 4-9 ppb) when average over the entire domain. The model runs start at midnight on the 31st. The x-axis denotes hours from the beginning of the simulation.

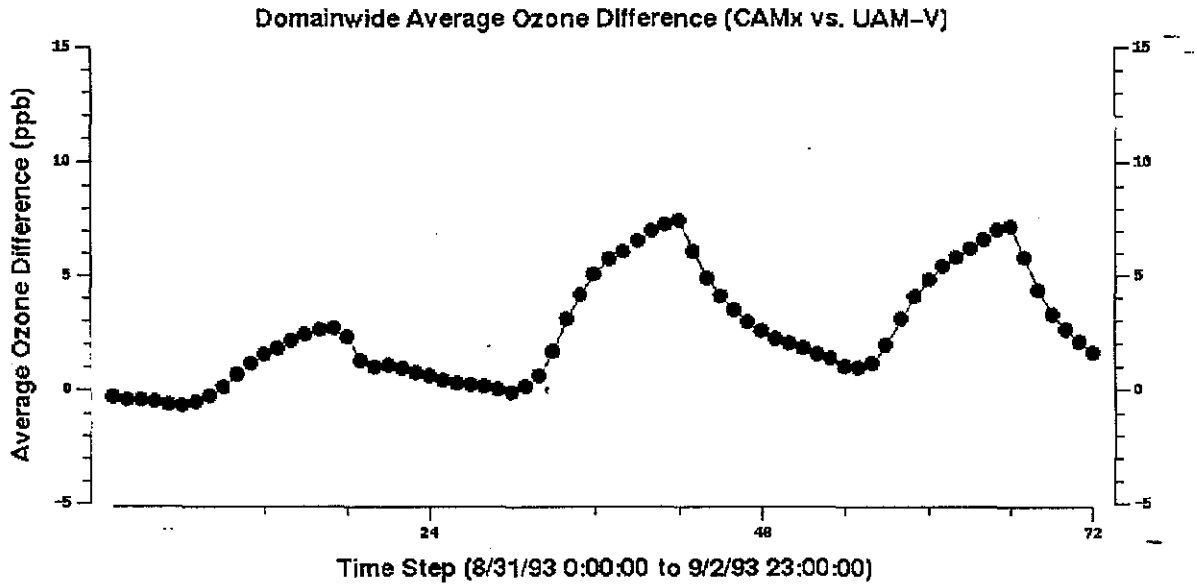

Figure 4-1. Domain-wide Layer 1 Average Ozone Difference (CAM_X vs. UAM-V)

There are 41 ozone sites within the COAST modeling domain. Appendix A contains a plot showing the location of these monitoring sites along with time series plots for each of these monitors comparing the ambient data with the CAM_X model predictions and the UAM-V model predictions. Ozone, NO, NO_2, and CO are compared and plotted at every location, even if that monitor only collects one species or contains missing data. The large majority of the sites show a pattern of higher afternoon ozone peaks in the CAM_X modeling with near-equal levels of predicted ozone at night. Peak afternoon ozone at individual sites can be 10-25 ppb greater in the CAM_X modeling.

4.1.1 Beaumont-Port Arthur area

There are seven monitoring locations in Jefferson, Orange, and Hardin counties: BMTC, S43S, PAWC, S40S, S42S, WORA, and KTZA. All seven of these stations show a consistent pattern of 10-20 ppb more ozone in CAM_X than in UAM-V on the afternoons of 9/01 and 9/02. At night and on the first day of the simulation (8/31), the models do not diverge greatly in their ozone predictions. In terms of NO_X species, UAM-V appears to maintain more NO and NO_2 during the early morning hours in the surface layer. For example, look at the S43S site (SETRPC SITE 43 TX). Starting around 4 a.m. on each of the three episode days, the model NO_2 traces start to diverge. From the animation of NO_2 differences, this effect appears to result from reduced NO_2 transport from the Houston-Galveston area (see web site). (It is possible that there is more deposition in some grid cells in the overnight hours in CAM_X. This explanation is consistent with model differences during other nighttime periods and is consistent with known model updates.) The CO concentrations between the two models are essentially identical, except for a plume impact at KTZA where UAM-V predicts about 200 ppb more CO.

Figure 4-2 shows the average difference between CAM_X and UAM-V over the Beaumont-Port Arthur area. Again, one can see the CAM_X surfeit in ozone during the afternoon and the CAMX deficit in NO_2 from sunset to sunrise. It appears that UAM-V maintains more NO_X in the surface layer overnight, especially downwind of urban areas.

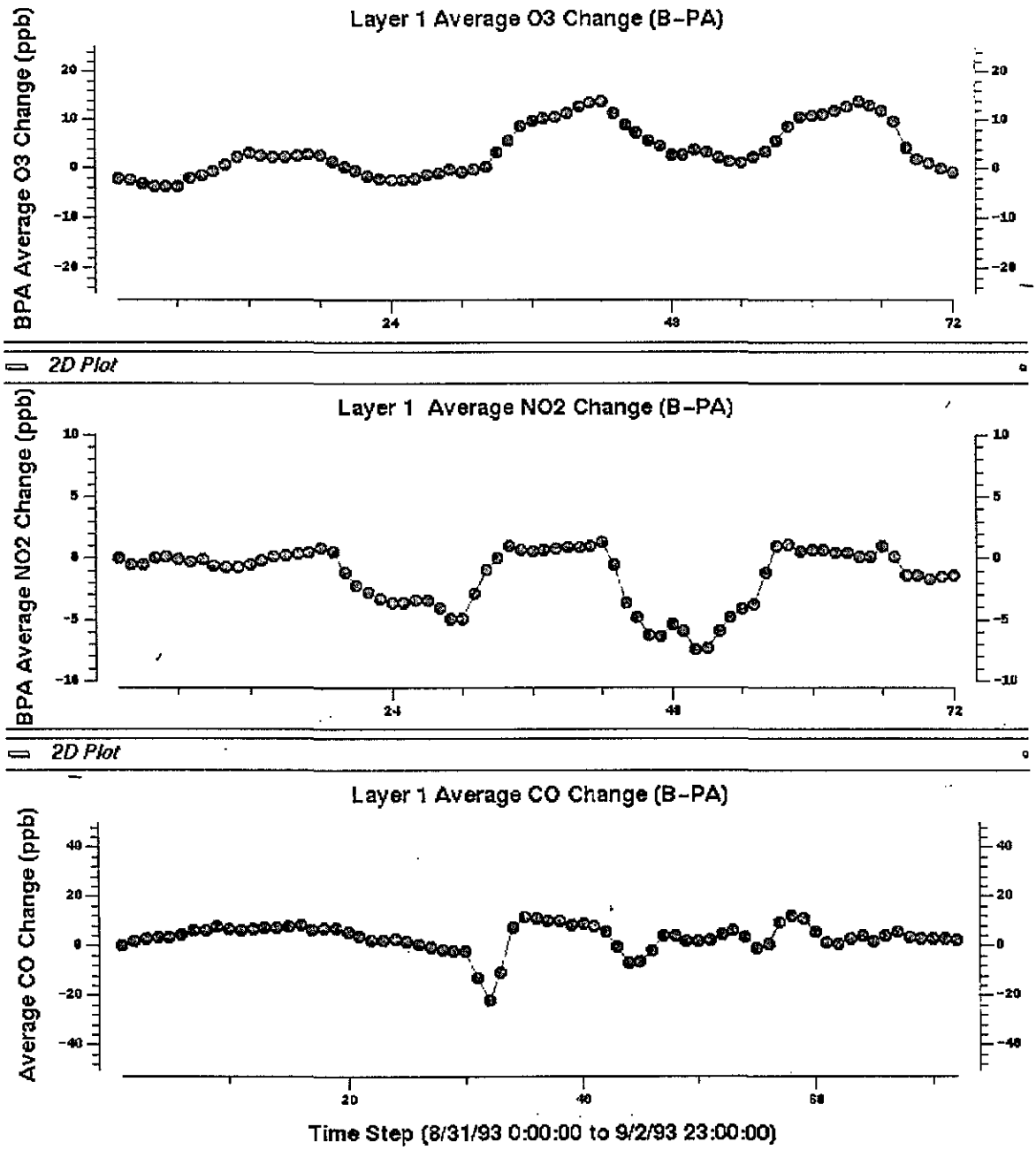

Figure 4-2. Beaumont-Port Arthur Layer 1 Average Ozone, NO_2 and CO Differences (CAM_X vs. UAM-V)

4.1.2 Southwest Louisiana area

There are four monitoring locations in Calcasieu and Beauregard counties in far Southwest Louisiana: VINL, CARL, WLKL, and RAGL. (The LEBL site is just out of the modeling domain.) Generally, the differences between the models in these two regions mirror the differences seen in the B-PA area. There is more model ozone in CAM_X over this region in the afternoon, on the order of about 10 ppb. There is less NO_X, especially late on the 1st and early on the 2nd. The VINL, CARL, and WLKL monitors all show a double-humped pattern of more NO_2 within UAM-V. Animations (and the lack of fresh NO at these times) indicate that there is less transport of NO_X from Beaumont-Port Arthur (first hump around 2100 on 1st) and from Houston-Galveston (second hump around 0300 on the 2nd) during this time span.

4.1.3 Galveston Bay area

For the purposes of this report, three ambient data sites were defined to represent the Galveston area as a whole: SWTC, SPTC, and SBRC. All three sites experienced high levels of ozone (model and observed) on the on 9/01/93. Once again the same CAM_X to UAM-V differences were noted. Simulated ozone was higher in CAM_X by about 10-20 ppb. NO_X was lower, especially during the overnight hours. The only difference is that NO levels were slightly different between the two models over this area near sunrise (0600 local time). There is more transport of NO from the E. Houston area in the UAM-V simulation.

4.1.4 Background areas

The CLTA, T04A, T21A, and VCTC sites were defined to be background type monitors for this analysis. They are background monitors in the sense that, for this episode, they do not appear to be affected by urban areas. The ozone traces (CAM_X versus UAM-V) are more similar than in other areas, but still exhibit about 3 to 6 ppb excess in CAM_X. The precursor traces are very similar, with the exception of the CLTA site in Brazoria County, which seems to be impacted by a local NO source.

4.1.5 Houston area

The sites in the Houston area exhibit a variety of signals when comparing between the two models. In general, there is more CO and NO_X resident in the CAM_X modeling from the transportation network and local Houston non-point emissions. For example, see C35C, H01H, H03H, H04H, HCFA, and HMCA. All of these are extremely urban locations as evidenced by the high NO concentrations and little to no ozone at night (observed and modeled). At these VOC-limited sites, model ozone is higher in UAM-V (especially on 9/01), because there is less titration of ozone as the NO is not as high.

There is a separate set of Harris County monitors (CRSC, H08H, H10H, H11H, and HCQA) which are outside the immediate urban core in a more suburban location. These sites show the opposite pattern when comparing the two sets of model output data. Ozone is higher

and NO_2 is lower during the peak afternoon hours in CAM_X. This signal is similar to the effects in B-PA, Southwest LA, and the Galveston Bay area.

4.2 CONTOUR PLOT AND ISOPLETH ANALYSES

Appendices B and C contain isopleth plots of CAM_X and UAM-V predicted ground level hourly ozone concentrations with observed concentrations overplotted. The plots were prepared for every third hour as well as for the hour of peak simulated ozone (1600 local time on all days). Solid line isopleths are plotted at 40 ppb intervals with dashed line isopleths every intermediate 10 ppb. Appendix D contains isopleth plots showing the difference between surface ozone between the two models for the same selected hours. Shaded isopleths mark those areas for which UAM-V predictions are higher than those from CAM_X. Differences are contoured at every 10 ppb. The maximum positive and maximum negative changes (UAM-V > CAM_X) are plotted in the lower right-hand corner of the plots.

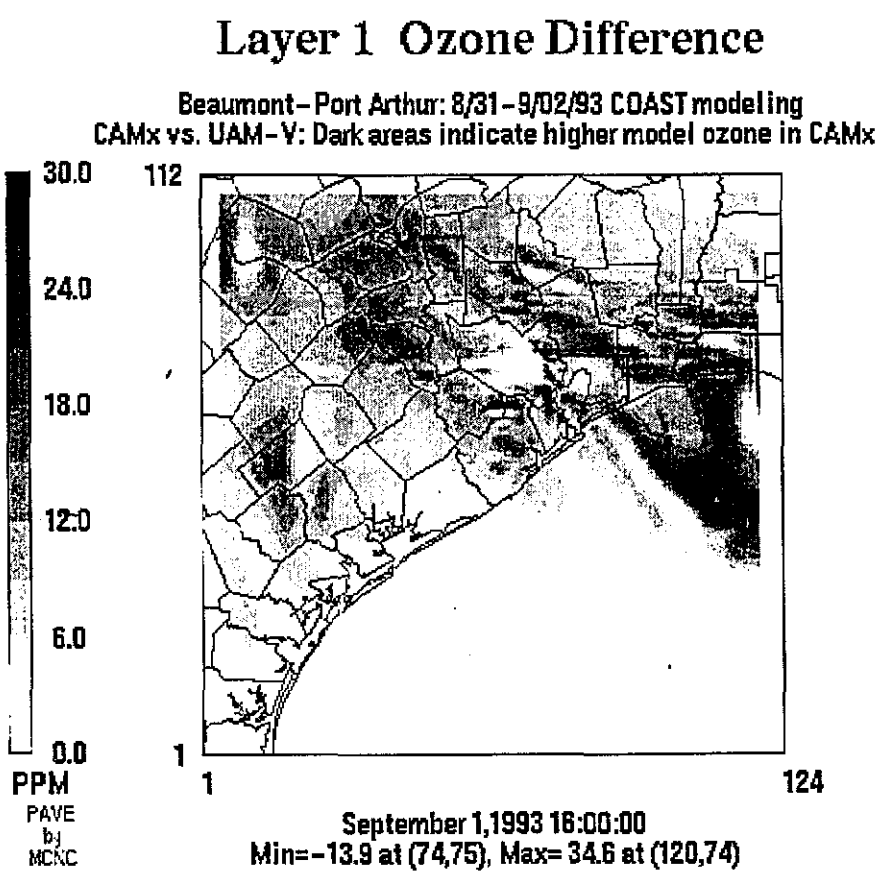

Figure 4-3. Ozone Difference between CAM_X and UAM-V base case simulations on the afternoon of 1 September 1993.

Figure 4-3 shows the ozone difference between the two models in the surface layer during the afternoon of September 1, 1993. The shaded portion of this plot indicates those areas in which the CAM_X model ozone exceeded the UAM-V model ozone for this hour. As can be

seen, a large portion of the domain contains higher concentrations of ozone in the CAM_X outputs for this representative hour. The maximum increase in ozone over the original UAM-V modeling is 34.6 ppb and occurs over the Gulf of Mexico. Most of the land portion of the domain experiences 3-9 ppb higher ozone in CAM_X.

Figure 4-4 displays those areas over which the UAM-V concentrations were greater than CAM_X. There is just a small area in the vicinity of downtown Houston and a few cells in San Jacinto County that meets these criteria. The largest negative difference (CAM_X < UAM-V) is over Houston and has a value of 13.9 ppb.

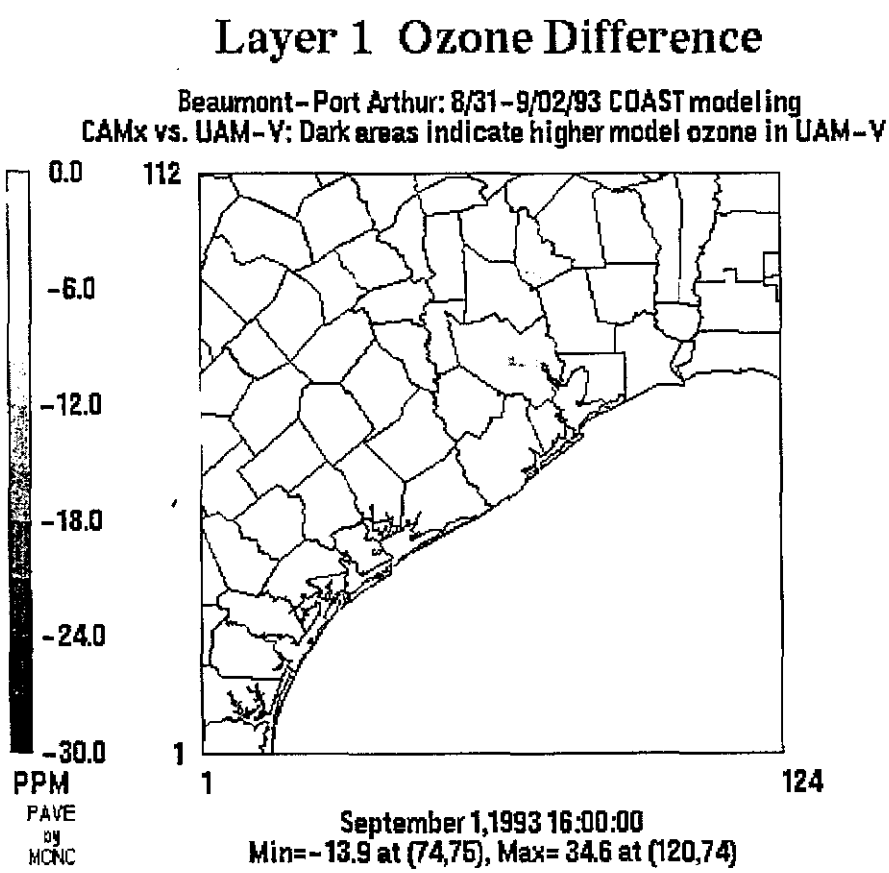

Figure 4-4. Ozone Difference between CAM_X and UAM-V base case simulations on the afternoon of 1 September 1993.

Several features are evident when one views the hourly differences in domain-wide ozone over the two models. Figure 4-5 shows the differences in the ground-level ozone fields at the end of the first hour. (Model outputs are written at an hourly frequency.) On the left half of the figure, the positive differences between CAM_X and UAM-V are plotted. The right half of the figure displays those grid cells in which UAM-V concentrations exceed that modeled in CAM_X. There appears to be some displacement in the initial ozone concentrations. As can be seen in

Figure 4-1 however, the net difference at the end of the first hour is near zero. These differences were determined to result from legitimate differences between the two models after one hour of simulation time, not the inadvertent use of differing initial condition files. One can note that the differences are greatest in the inner 4km grid. This may indicate that the interpolation (coarse to fine grid) methods differ in the two models, as the initial condition data is only input into the coarse grid.

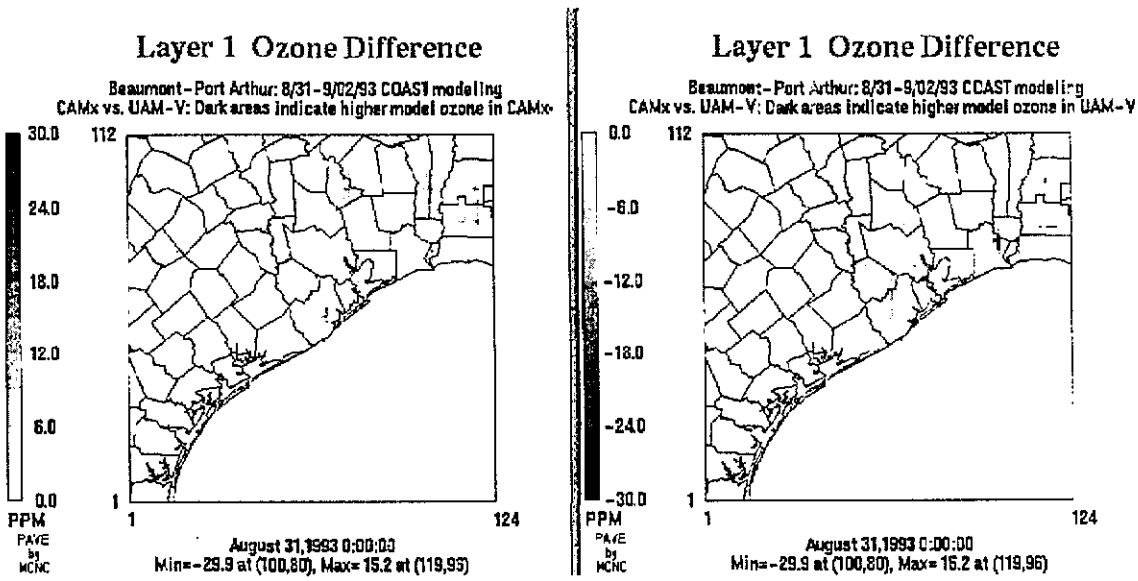

Figure 4-5. Ozone Differences between CAM_X and UAM-V base case simulations after one hour model time. Left half of plot shows areas in which CAMx is greater than UAM-V. Right half of plot shows areas in which UAM-V is greater than CAMx.

A second interesting pattern that stands out in the hourly ozone difference plots is the existence of difference "plumes". For example, Figure 4-6 shows the surface ozone difference field for four hours on 2 September 1993. Note that at 0900 much of the ozone increase in CAM_X, especially over the 4-km fine grid, appears to take the form of distinct individual plumes (e.g., off Galveston Bay in Chambers County or in south central Brazoria County). The most distinct plume of CAM_X surplus ozone appears to be emanating from a point near Booth TX, in Fort Bend County. By 11 a.m., the difference pattern still has distinct plume-like features. The area of increased ozone downwind of the Fort Bend County source and the northern tip of Galveston Bay source merge together over the Gulf of Mexico. Similar plumes of increased ozone are seen in the Beaumont-Port Arthur area. By 1 p.m. the areas of higher ozone produced in plumes downwind of major NOx sources have diffused to the degree that individual plumes are not as evident. By 3 p.m., near the hour of highest ozone, there is a large area of CAMx-enhanced ozone (around 20 ppb) being advected ashore just east of Port Arthur, TX. It is speculated that differences in the treatment of subgrid scale plumes are the cause for some of the largest ozone differences between the two models.

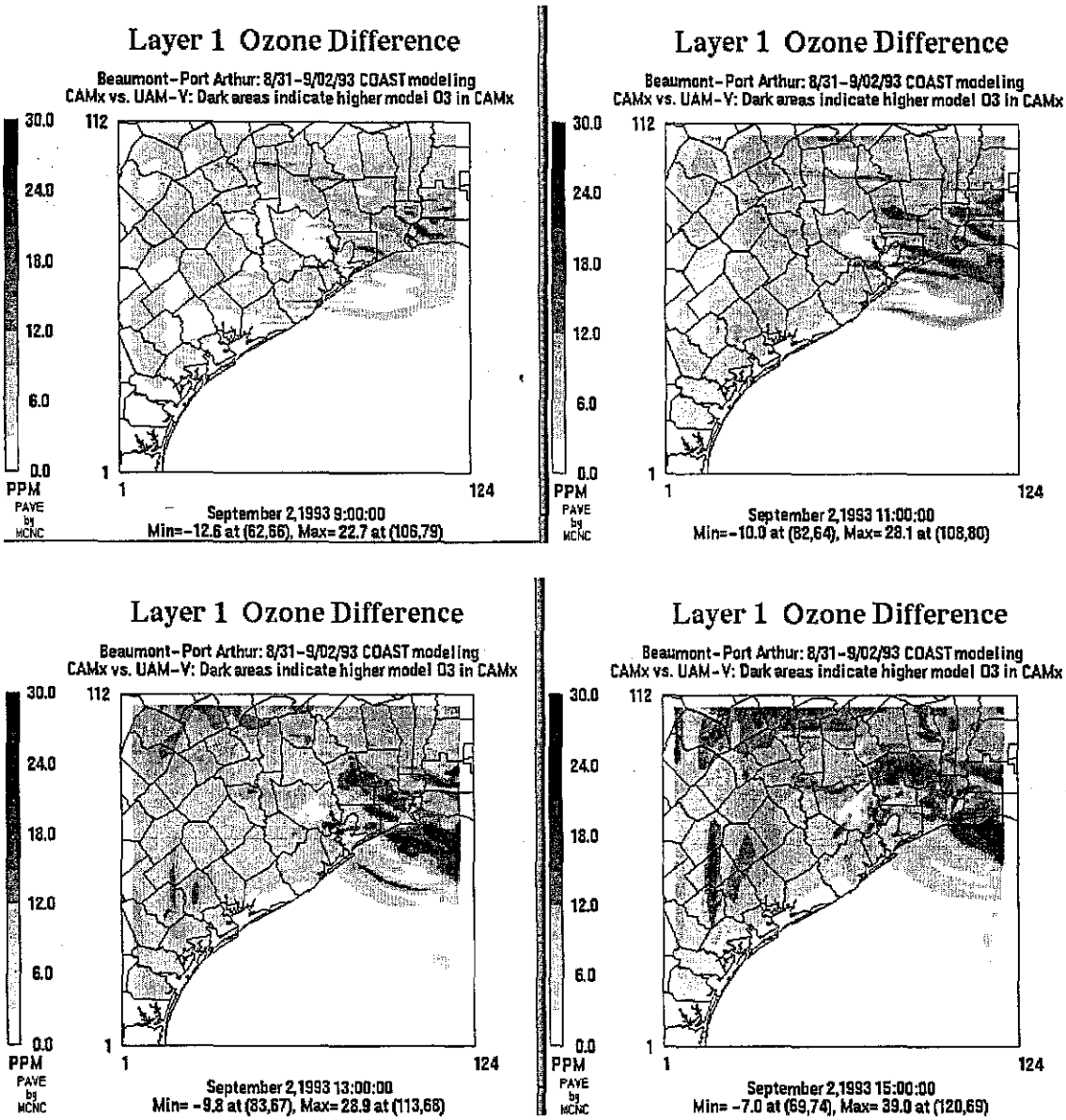

Figure 4-6. Ozone Differences between CAM_X and UAM-V base case simulations for four hours (0900, 1100, 1300, and 1500 local time) on 2 September 1993.

One of the major differences between the CAM_X and UAM-V software is in the Plume-in-Grid (PiG) methodologies. According to the CAM_X User's Guide (Environ, 1997), the primary advantage of the CAM_X PiG module is the computational savings. The CAM_X model uses a highly simplified set of chemical reactions in the sub-grid scale plume model compared to UAM-V. Additionally, the criteria that govern when parts of the plume mass are dumped to the model grid have changed substantially in CAM_X. According to the CAM_X model developers, there is considerable uncertainty in the algorithms that govern the mixing of plume mass to the grid.

Another interesting feature from the hourly comparisons of surface ozone concentrations in the two models is the frequent occurrence of a box shaped pattern in the ozone difference contours. These linear features are co-located with the interface between the coarse and fine grids. For instance, in Figure 4-7 one can detect parts of the western and southern faces of the 4km fine grid. Analysis of the ozone fields within each of the individual models does not reveal "box-like" patterns in the base case ozone. In Figure 4-7, CAM_X generates more ozone (relative to UAM-V) in the interface cells than in the cells on either side of the boundary, but this is not a consistent effect. In general, the "box-like" patterns are more evident in the Houston-Galveston episode than this one.

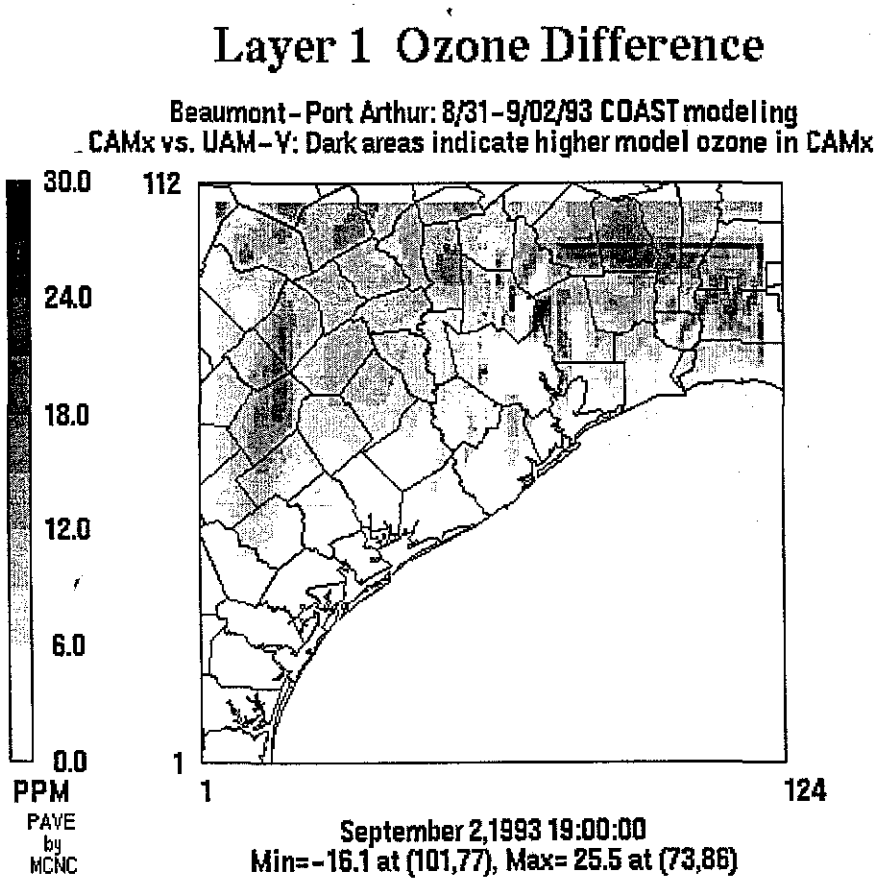

Figure 4-7. Ozone Differences between CAM_X and UAM-V base case simulations at 1900 local time on 2 September 1993.

4.3 STATISTICAL ANALYSES

Table 4-1 shows the performance statistics for ozone for the six-day episode for each of the model simulations. The CAM_X results tend to exhibit more of an overprediction bias than was seen in UAM-V. Normalized bias values range from about 2 percent to 21 percent. The gross error is very slightly larger in the CAM_X runs as well.

Unpaired peak prediction accuracy is better in the CAM_X runs than in their UAM-V counterparts ranging from 5 overprediction to 3 underprediction. (Note: the first day of the simulation could be treated as a ramp-up day.) All of the values, in both models, meet the broad USEPA criteria for successful model performance.

Table 4-1. Model ozone performance statistics. Numbers in bold are CAM_X.

Date	# of pairs	Max. Obs. (ppb)	Max. Stn. Wide Sim. (ppb)	Max. Dom. Sim. (ppb)	Acc. Peak	Avg. Acc. Peak	Norm. Bias	Gross Error	Avg. Sim. (ppb)	Avg. Obs. (ppb)
8/31/93	15	96	**88.7**	**100.4**	**4.6**	**-12.7**	**-16.9**	**31.4**	**60.2**	75.0
			86.4	102.5	6.8	-13.1	-21.2	31.1	57.2	
9/1/93	76	164	**143.8**	**172.7**	**5.3**	**17.1**	**17.7**	**30.7**	**94.2**	84.3
			151.5	154.9	-5.5	12.1	9.2	29.7	87.3	-
9/2/93	96	139	**128.7**	**134.1**	**-3.6**	**-0.6**	**2.7**	**17.8**	**82.2**	81.8
			117.9	128.7	-7.4	-10.8	-11.0	17.9	71.4	

The important issue at this point is not how well any particular model performs relative to a separate model. Considerably more analysis above and beyond simple ozone performance statistics would be required to make such value determinations. Of more interest at this stage of the B-PA modeling is the similarity in model performance between UAM-V and CAM_X. Considering the values within Table 4-1 and in Figure 4-8, it appears that the ozone differences observed in the isopleth and time series plots do not translate to drastically different model performance statistics. Certainly, ozone is higher within the CAM_X simulations when the domain is viewed as a whole (urban sites are the exception to this rule) and this translates to more of a positive bias for surface ozone. However, the gross error in surface ozone is essentially identical between the two runs and the unpaired peak prediction accuracy is somewhat better in the CAM_X simulations than was previously seen in UAM-V. In fact, unlike any of the 6 episode days in the Houston-Galveston comparison (MCNC, 1999), CAM_X clearly performs better than UAM-V for 2 September 1993.

Both sets of simulation results appear to be plausible base cases based on a preliminary assessment of model performance. The B-PA modeling protocol calls for the completion of a more detailed performance evaluation in later stages of the project.

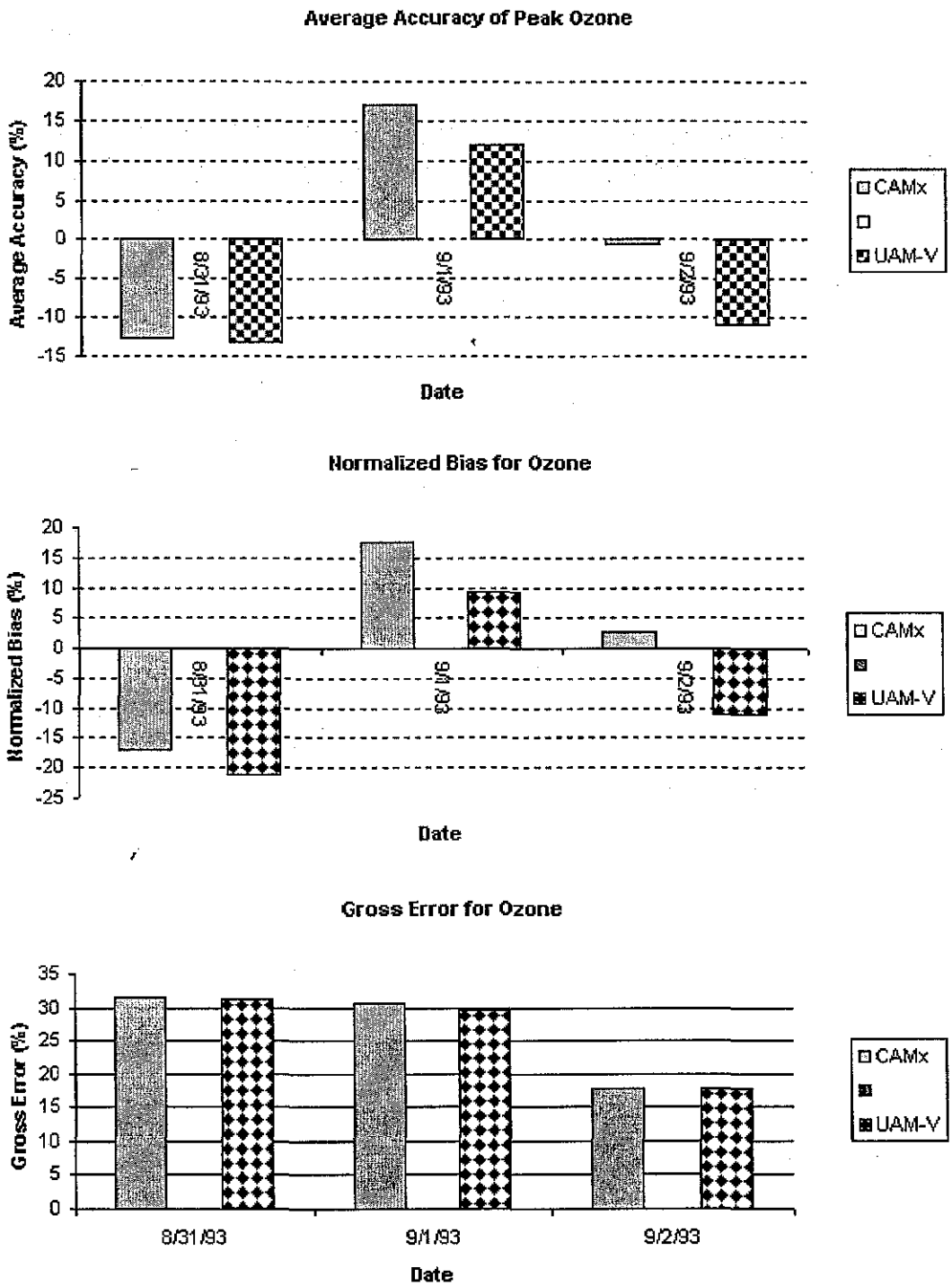

Figure 4-8. Model Performance Statistics for Surface Ozone in CAM_X and UAM-V. Accuracy of Peak Predictions, Normalized Bias, and Gross Error are the three metrics considered.

5. CONCLUSIONS

As has been seen in previous comparisons of CAM_X and UAM-V model output, the CAM_X model generally produces more ozone over the domain. When averaged over the entire COAST domain for the 31 August -- 2 September 1993 episode, the CAM_X model ozone concentrations are generally 3-7 ppb higher than UAM-V. Interestingly, the differences between the two models for ozone and ozone precursors varied as a function of proximity to the urban core. In the most urban sites, CAM_X tended to be even more radical-limited than UAM-V over those areas (i.e., Houston grid cells had more NO and less ozone). Along the periphery of the city there was a zone in which the two models produced essentially identical traces. Beyond that, in the suburban and rural regions, the signal switches to higher simulated ozone values in CAM_X.

Ideally, these two models would be instrumented with process analysis. That would allow one to compare differences in the individual terms (chemistry, advection, diffusion, deposition, etc.) between the two models. In the absence of that capability, one can only make educated guesses as to the causes of the difference between CAM_X and UAM-V. In all, four potential causes for the differences in pollutant concentrations have been hypothesized:

1) There are known differences in the formulations of CAM_X and UAM-V. For instance, the treatment of deposition has been improved within CAM_X. Most importantly, the chemical solver in CAM_X has been modified to become more flexible (easier to upgrade code when chemical mechanism is revised) and computationally efficient. In particular, the differences between the model behavior in urban versus rural areas may indicate that the chemistry term of the species continuity equation has changed significantly.

2) Treatment of point source plumes differs between the two photochemical models. CAM_X appears to dump point source NO_X closer to the source. This appears to result in more favorable VOC/NO_X within plumes emanating from large NOX sources.

3) There appear to be differences in the algorithms governing transfer of mass between the coarse and fine grids in the two models. While neither model features "box-like" ozone patterns along the interface between the coarse and fine grids, the ozone difference plots often feature such a pattern.

4) Differences occur in the first hour of the simulation. The model output data diverge especially strongly over the nested grid. It looks as if the 16km initial condition file is interpolated slightly differently between the models. This has little overall effect on the modeling, as the total mass being initialized is almost exactly equal.

Even with the deviations in model output, the difference in model performance between the two models was determined to be fairly small over the B-PA airshed for the 31 August -- 2 September 1993 COAST episode. The mean normalized bias for those observed-model pairs greater than 60 ppb is slightly more biased than what was previously seen in the UAM-V

modeling on 2 of the 3 days. The error and accuracy values are more closely aligned between the two sets of results. All surface ozone statistics (for non-ramp-up days) fell within USEPA acceptability criteria. A cursory evaluation of model performance indicates that both the UAM-V and CAM_X results are plausible base cases. In a general sense the model predictions are largely comparable across the 2 models. It is unlikely that one model would require a *significantly different control strategy than the other, in terms of magnitude or type of emissions* controls.

6. REFERENCES

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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.