Final Report

UPDATED BOUNDARY CONDITIONS

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Prepared for

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EXECUTIVE SUMMARY

Boundary conditions play an important role in grid modeling. They represent all emissions released outside of a modeling domain that can be transported into the domain. ENVIRON previously developed boundary conditions for the TCEQ 36 km domain by performing CAMx simulations for a continental-scale 36 km domain (Figure ES-1) used by several Regional Planning Organizations (RPOs). Boundary conditions for the RPO domain were, in turn, extracted from two global models – MOZART and GEOS-Chem.

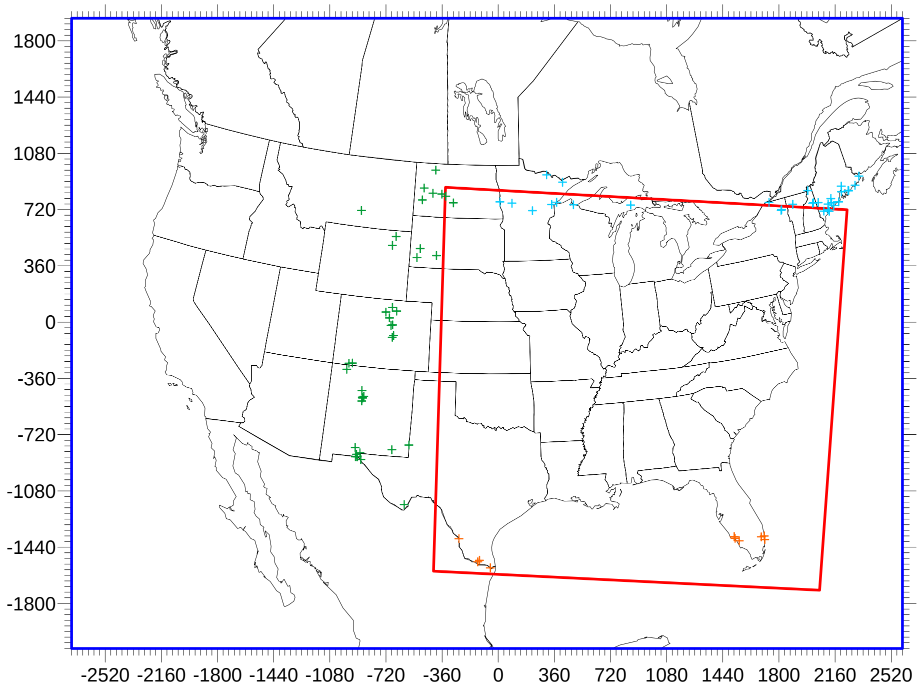


Figure ES-1. Map of the national RPO 36 km domain, the TCEQ's eastern US 36 km domain, and ozone monitoring locations near the TCEQ domain boundaries.

This project developed new boundary conditions for the TCEQ domain for the summers of 2005 and 2006. The TCEQ boundary conditions were extracted from CAMx runs on the RPO domain, which used boundary conditions from date-specific GEOS-Chem and date-specific MOZART. The GEOS-Chem results used in this study were specifically for 2005 and 2006 whereas previously monthly averaged 2002 results had been used.

Model performance at ozone monitoring sites near the TCEQ domain boundaries (marked in Figure ES-1) showed that date-specific 2005/6 GEOS-Chem results produced more ground-level ozone than MOZART on all lateral boundaries, and even more ozone than the 2002 monthly averaged GEOS-Chem results used previously. This trend is also reflected in RPO lateral boundary contributions to ozone in Houston, shown in Figure ES-2. Date-specific GEOS-Chem consistently performed better than both MOZART and the 2002 monthly-averaged GEOS-Chem near the western boundary. Performance near the southern boundary was either mixed or tended to favor MOZART. The TCEQ boundary conditions extracted from the date-specific GEOS-Chem runs are worthy of further evaluation.

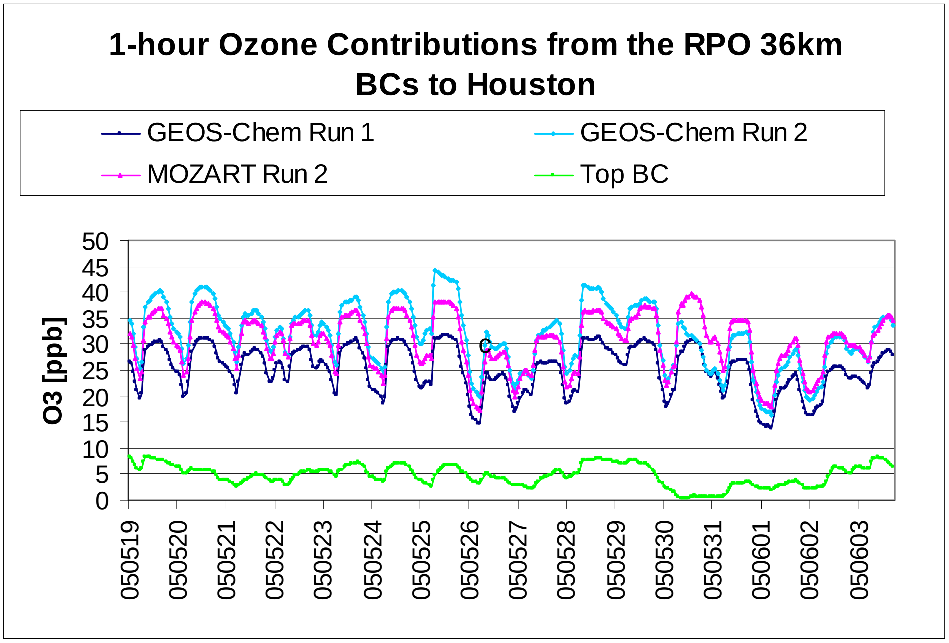


Figure ES-2. Time series of ozone contributions to Houston from the RPO 36 km domain boundaries

TCEQ domain boundary conditions for the 2018 future year were updated with 2005/2006 date-specific GEOS-Chem boundary conditions. Differences between the base and future year runs are attributed to changes in anthropogenic emissions and differences from date-specific (base year) and typical fire emissions (future year). The date-specific NCAR fire emissions generated more ozone than the typical fire emissions in Houston during most hours of the episode dates. Most differences in Houston were less than 1 ppb, but there were spikes of up to 7 ppb difference. Caution may need to be exercised when mixing the two fire inventories when conducting design value scaling for the Houston ozone monitors.

1.0 INTRODUCTION

Boundary conditions are used to represent emissions released outside of a modeling domain that can later be transported into the domain. The TCEQ 36 km modeling domain covers most of the central and eastern US, but excludes the western US along with most of Mexico and Canada. To address emissions outside the domain that can be transported into the TCEQ domain, boundary conditions were extracted from CAMx runs on the Regional Planning Organizations' (RPO) continental-scale 36 km domain.

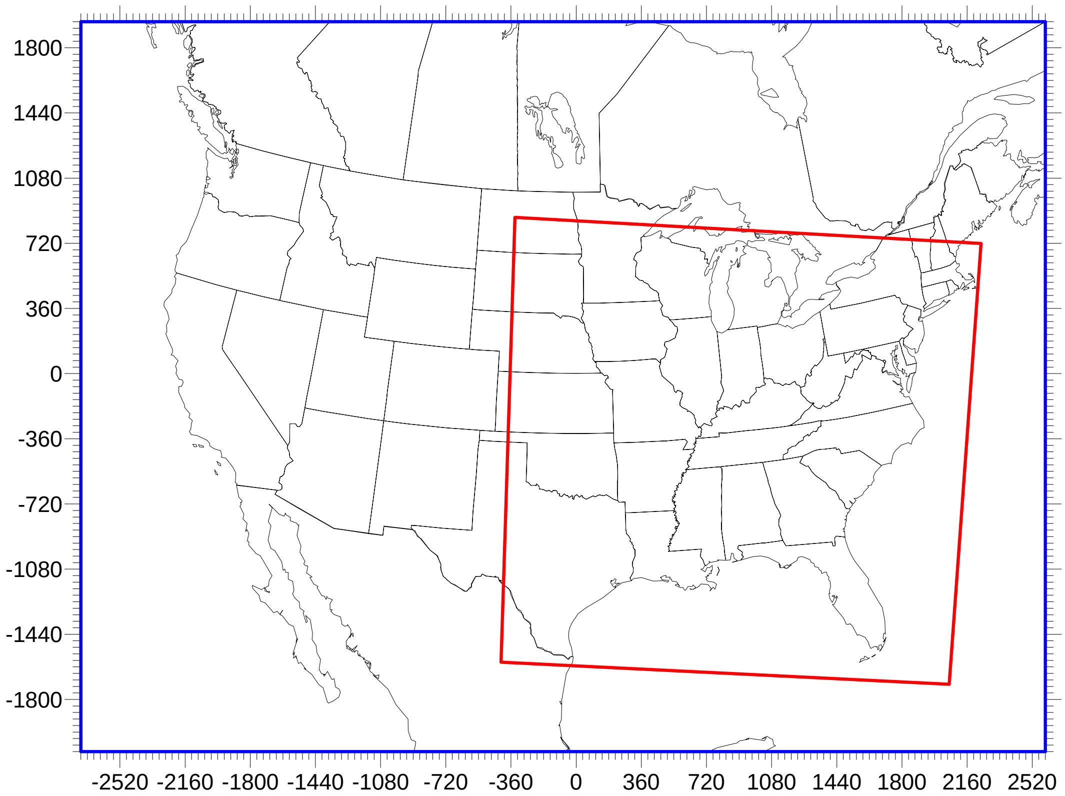
In 2008, ENVIRON ran CAMx on the RPO domain for the summers of 2005 and 2006, which contain five episode periods to be used for SIP modeling of the Houston/Galveston/Brazoria (HGB) non-attainment area (Tai, 2008). Two CAMx runs were performed for each summer. One used RPO domain boundary conditions extracted from the GEOS-Chem global model; the other run, from MOZART. Ozone model performance was evaluated at surface monitoring sites near each of the TCEQ 36 km lateral boundaries to determine which CAMx run produced better performance for the TCEQ domain. The run with MOZART boundary conditions tended to perform better possibly because the MOZART outputs were date-specific for 2005 and 2006 whereas the GEOS-Chem outputs were 2002 monthly averages.

In this project, date-specific 2005 and 2006 GEOS-Chem outputs were obtained. CAMx runs were updated with the date-specific GEOS-Chem boundary conditions for the summers of 2005 and 2006. Section 2 compares the model performance near the TCEQ boundaries when using date-specific GEOS-Chem to runs using MOZART, and monthly averaged GEOS-Chem boundary conditions.

Section 3 describes updated 2018 future year CAMx runs using date-specific GEOS-Chem boundary conditions. The only differences between the base year and 2018 future years are the anthropogenic emissions and fire emissions. In the 2008 study, two sets of fire emissions were generated. In the 2005 and 2006 base years, fire emissions were based on date-specific NCAR satellite-data; in 2018, fires emissions were based on the CENRAP 02g typical fire emissions inventory. An analysis of fire emissions is included to address the usage of different fire emission inventories.

2.0 CAMx BASE YEAR MODELING

In 2008, ENVIRON (Tai et al., 2008) performed CAMx simulations of the continental-scale RPO domain, which covers the entire continental US and large sections of Canada and Mexico, and includes the entire TCEQ 36 km domain when transposed to the RPO projection, as shown in Figure 2-1. Boundary conditions for the TCEQ domain could then be extracted from the CAMx outputs of the RPO run to account for emissions outside the TCEQ domain, including fires from the western US.



RPO 36 km **(center 40N, 97W; true lats 33N, 45N)**
148 x 112 (-2736, -2088) to 2592, 1944)

TCEQ 36km **(center 40N, 100W; true lats 30N, 60N)**
69 x 67 (-108, -1584) to (2376, 828)

Expressed in the RPO projection:
SW: (-414.84, -1593.96)
SE: (2060.40, -1715.88)
NE: (2236.80, 719.28)
NW: (-338.28, 862.74)

Figure 2-1. Map of the national RPO 36 km domain with the TCEQ eastern US 36 km domain

CAMx was run from May 1 to September 1, 2005 and May 1 to October 15, 2006, covering the five high ozone episodes in the Houston/Galveston/Brazoria (HGB) non-attainment area with at least 18 days of model spinup for each episode:

- May 19 – June 3, 2005
- June 17 – 30, 2005
- July 26 – August 8, 2005
- May 31 – June 16, 2006
- August 1 – October 15, 2006

Lateral boundary conditions for the RPO domain were extracted from two global models – the Model for Ozone And Related chemical Tracers (MOZART; Horowitz et al., 2003) and the Goddard Earth Observing Systems Chemistry (GEOS-Chem; Bey et al., 2001). Boundary conditions were extracted from date-specific MOZART outputs, provided by Louisa Emmons at NCAR, and existing 2002 monthly averaged GEOS-Chem outputs since date-specific GEOS-Chem outputs were not available. Model performance was evaluated at surface ozone monitoring sites near the TCEQ 36 km northern, western, and southern boundaries to determine which global model yielded better results.

In this task, date specific GEOS-Chem outputs were obtained for both the 2005 and 2006 episodes. CAMx was rerun for the RPO domain using the updated GEOS-Chem outputs as boundary conditions, and compared to the runs using MOZART and original GEOS-Chem boundary conditions. All runs were run in GMT.

2.1. CAMx INPUTS

All CAMx inputs were unchanged from the 2008 runs except for the boundary conditions and a correction to the fire emissions. Meteorological inputs, photolysis rates, and the albedo/haze/ozone files were the same, and are described in the 2008 report (Tai et al., 2008).

Emission Update

In the 2008 runs, the 2005 and 2006 base year emissions were estimated by time-interpolating existing WRAP 2002b and 2018 inventories for all emission components except biogenics and fire emissions. These emissions were speciated to CB-IV. Date-specific biogenics and fire emissions speciated to CB05 were prepared using MEGAN version 2.1 and EPS3, respectively, and were added to the time-interpolated WRAP emissions.

Fire emissions were updated to account for time zone differences that affect the vertical distribution of emissions in the PSTFIR module of EPS3. The total fire emissions within each vertical column and hour were unaffected

Boundary Condition Update

In work performed in 2008, the 2005 and 2006 CAMx boundary conditions were extracted from date-specific MOZART outputs and from 2002 monthly-averaged and diurnally varying GEOS-Chem outputs.

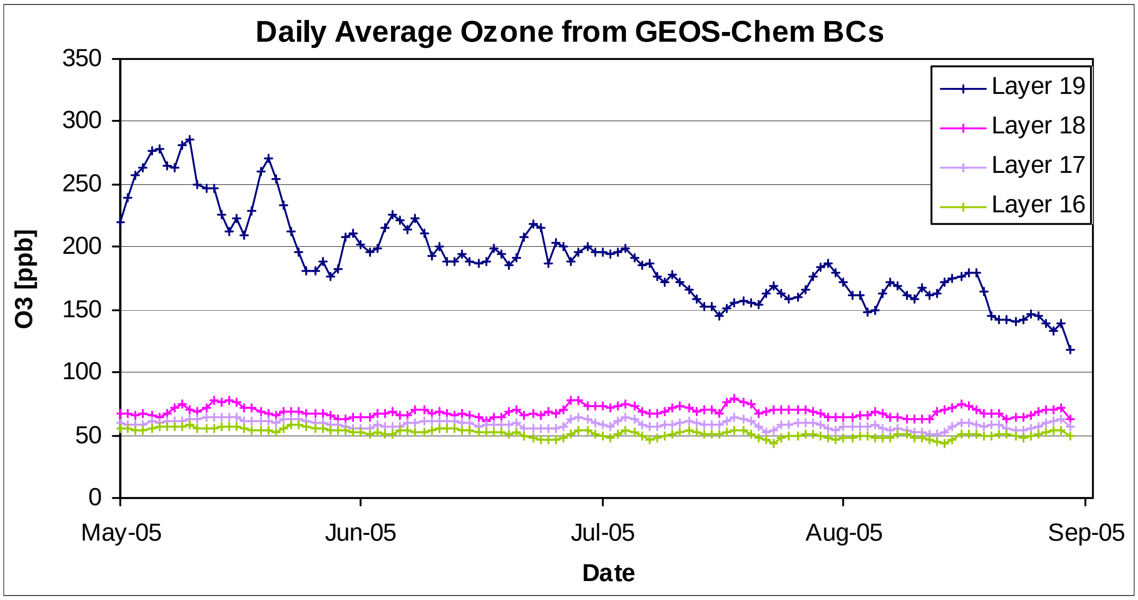
In this task, 2005 and 2006 date-specific GEOS-Chem outputs were obtained from Greg Osterman at NASA. Table 2-1 shows how the GEOS-Chem species are mapped to CAMx CB05 species. Fewer species are in the 2005 and 2006 files than in the 2002 GEOS-Chem, which included extended aerosol species. Data was available in 3-hourly intervals.

Table 2-1. Mapping of GEOS-Chem to CAMx CB05 species.

CAMx	GEOS-CHEM
NO2	NOx
O3	Ox - NOx
CO	CO
NXOY	2 N2O5
HNO3	HNO3
PNA	HNO4
H2O2	H2O2
NTR	R4N2
FORM	CH2O
ALD2	0.5 ALD2
ALDX	RCHO
PAR	0.333 PRPE + ALK4 +0.5 C3H8 + ACET + MEK + RCHO
OLE	0.333 PRPE
ETHA	0.5 C2H6
MEPX	MP
PAN	PAN
PANX	PPN + PMN
ISOP	0.2 ISOP
ISPD	MACR + MVK
SO2	SO2 + DMS
NH3	NH3
ISP	0.2 ISOP
PSO4	SO4 + MSA

A new version of GEOS2CMAQ (version 3.0) was used to map the GEOS-Chem outputs to CMAQ boundary conditions for the 19 layer RPO domain. The CMAQ2UAM converter linearly interpolated the 3-hourly CMAQ boundary condition file to hourly CAMx boundary conditions.

Figure 2-2 displays the daily average ozone at the boundaries of the four highest layers; layer 19 contained stratospheric ozone that was approximately 3 times larger than in the other layers. To reduce the stratospheric ozone impact, layer 17 boundary conditions were mapped to layers 18 and 19, as had been done with MOZART and 2002 monthly averaged GEOS-Chem boundaries.



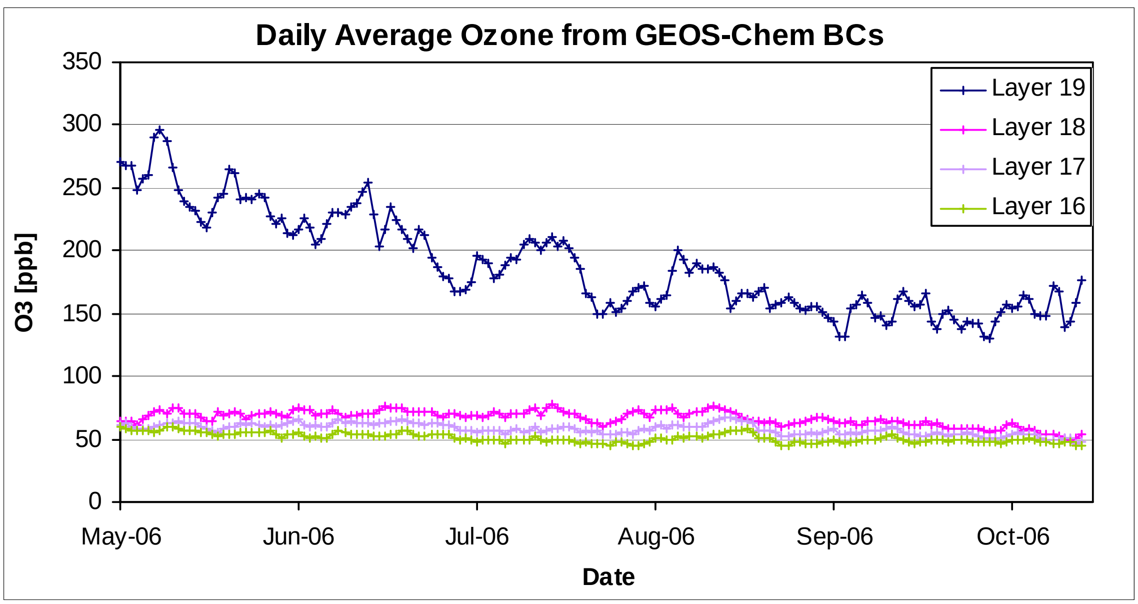


Figure 2-2. GEOS-Chem daily average ozone at the lateral boundaries of the top four layers in 2005 (top) and 2006 (bottom).

Two base year runs were updated for the summers of 2005 and 2006 using CAMx version 4.51. One run used MOZART boundary conditions with corrected fire emissions. The second run incorporated date-specific GEOS-Chem boundary conditions with updated fire emissions. For simplicity, these updated runs will contain a “Run2” extension; previous runs will hereafter be labeled “Run 1.” Three-dimensional outputs were generated so that boundary conditions could be extracted for the TCEQ 36 km domain.

2.2. CAMx OUTPUTS

Boundary Condition Extraction

Lateral boundary conditions for the TCEQ 36 km domain were extracted from CAMx outputs of the RPO domain. The extraction consisted of three steps. First, the three-dimensional outputs were reprojected from the RPO projection to the TCEQ projection. Each layer was interpolated and windowed to the new projection; then, the 19 vertical layers from the RPO configuration were mapped to TCEQ's eastern US 17 layer structure. Next, boundaries were extracted using the bndextr program, and then time shifted from UTC to CST. Boundary conditions were extracted for all five TCEQ episodes in 2005 and 2006 from both updated MOZART and GEOS-Chem runs.

Table 2-2 lists the reference state heights of the RPO vertical layer interfaces, assuming a sea level pressure and temperature of 1000 mb and 300K, respectively, and a temperature lapse rate of 50K when the pressure changes by a factor of e. Table 2-2 also lists the TCEQ 36 km domain's vertical layer interfaces, obtained from http://www.tceq.state.tx.us/implementation/air/airmod/data/hgb8h2/hgb8h2_camx_domain.html#layer, showing the RPO layer used to represent each of the 17 TCEQ vertical layers. All RPO layers were used except layers 3 and 12.

Table 2-2. Height interfaces of the RPO and TCEQ vertical layer structures.

Layer	RPO Height [m]	TCEQ 36 km Height[m]
19	16350	15179
18	8951	9167
17	5661	5836
16	3776	4106
15	2693	3026
14	1999	2103
13	1530	1353
12	1170	
11	995	1068
10	822	791
9	653	610
8	486	520
7	403	432
6	321	344
5	240	257
4	159	171
3	119	
2	79	85
1	40	34
0	0	0

Model Performance

Ozone model performance was evaluated at sites near the TCEQ 36 km boundaries to determine whether MOZART or GEOS-Chem yielded better boundary conditions for the TCEQ domain. Ozone data from EPA's Air Quality System (AQS) were formatted for the sites shown in Figure 2-3. All observations were time shifted to CST and were compared to CAMx outputs in the first layer, which were also time shifted to CST.

Evaluations were performed for sites along each boundary. The western boundary monitors (green) consisted of 39 sites located mostly in New Mexico, Colorado, and the Dakotas. The northern boundary sites (blue) contained 31 monitors, of which half were in Maine. The southern boundary sites (orange) had 10 monitors in southern Texas and Florida. Sites easily identified to be in urban cores, such as Miami, Denver, Albuquerque, and El Paso, were removed. The eastern border contained no sites since it was over the Atlantic.

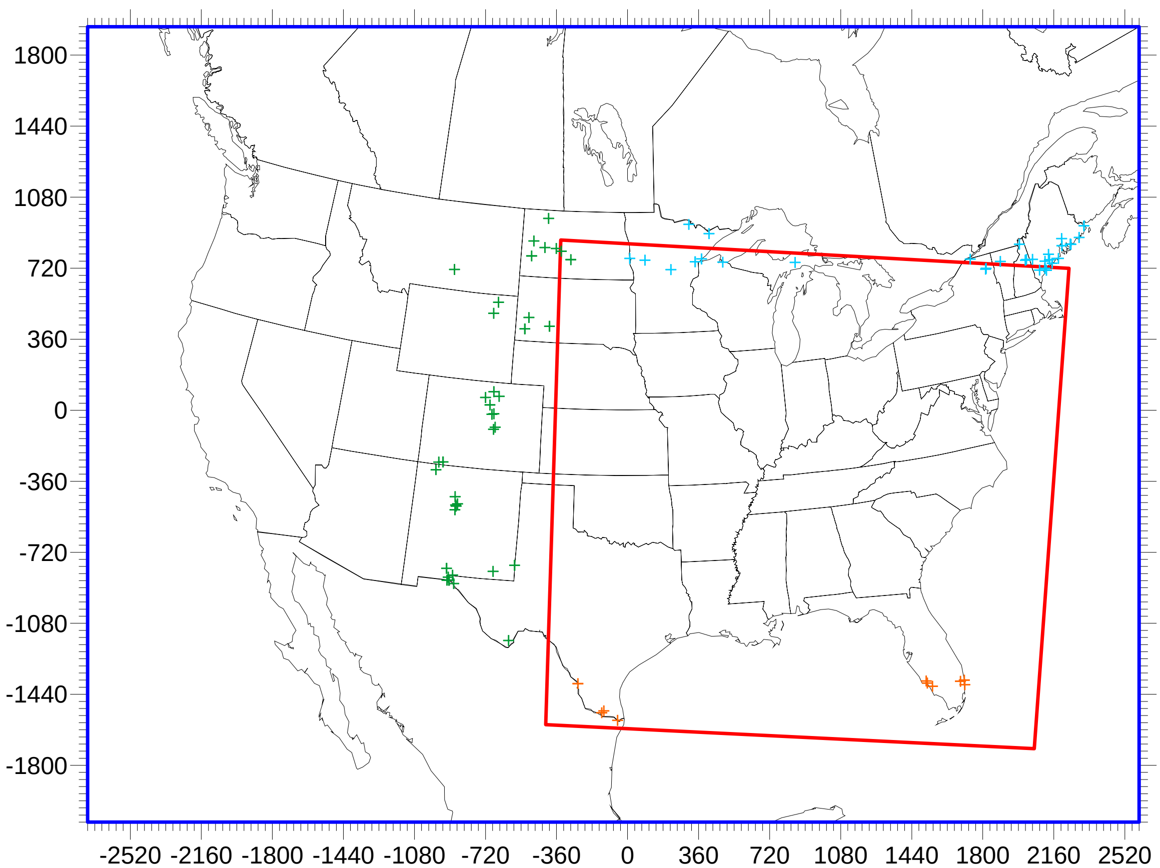


Figure 2-3. Map of AQS ozone monitoring sites near the TCEQ 36 km boundary.

<u>Updated MOZART Run</u>

The updated CAMx run of the RPO domain using MOZART boundary conditions (Run 2) was compared to the original MOZART run (Run 1) to quantify the impacts from the

NCAR satellite-derived fire emissions update. Both runs used date-specific MOZART boundary conditions. An analysis between the two runs was performed on the TCEQ western boundary since the western US had the most fire emissions. Figure 2-4 displays vertical cross sections of the TCEQ 17-layer western boundary. The x-axis shows the western boundary from Mexico on the left to North Dakota on the right; the y-axis shows the 17 vertical layers. Plots in the left and right columns show the largest increase and decrease, respectively, to hourly ozone in each of the five episodes resulting from the emissions update. Shades of red represent the largest differences.

The fire emissions update generally produced small differences to the western boundary. The May and June 2005, and June 2006 episodes showed the smallest changes as western boundary ozone differed less than ±2 ppb in almost all grid cells and hours in each episode. The August to October, 2006 episode had the largest differences, increasing 8ppb in the upper layers over South Dakota at 11AM on September 13, and over 3 ppb on September 7 (also at 11 AM) over Nebraska. Impacts from the latter propagated downward to generate a large area of ozone increases greater than 1 ppb in the episode.

Most of the increases were in the upper layers while more reductions were closer to the ground. This was expected since the time shift update would have aligned the higher emission rates in the daytime with more elevated plumes, based on the WRAP diurnal fire profile and buoyancy efficiency tables incorporated into EPS3 (WRAP, 2005).

Figure 2-5 compares the daily 1-hour ozone normalized bias and error between the two MOZART runs at the 39 sites near the TCEQ western boundary for the May, 2005 episode. Statistics showed little change due to the small differences close to the ground.

In the other episodes, the MOZART Run 2 statistics also showed little change from MOZART Run 1. Bar charts displaying the normalized bias and normalized error for all episode dates can be found in Appendix A. Although MOZART boundary conditions were used to evaluate the impacts of the emissions update, the fire emissions update should also have a negligible impact when using GEOS-Chem boundary conditions.

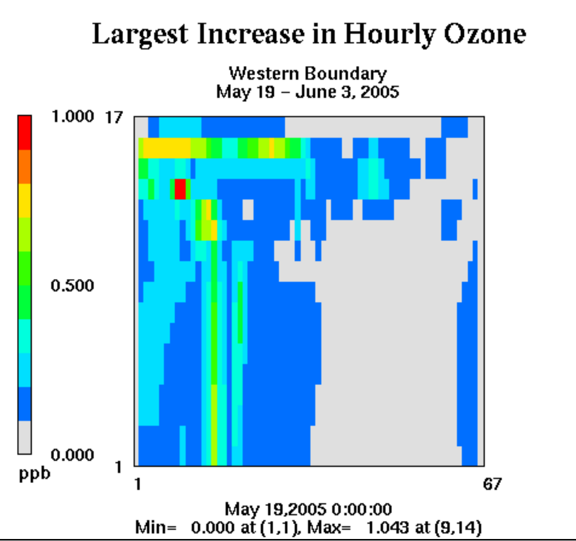
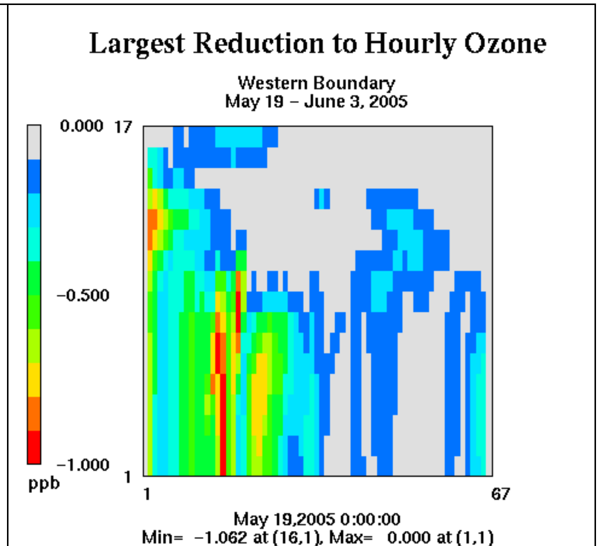
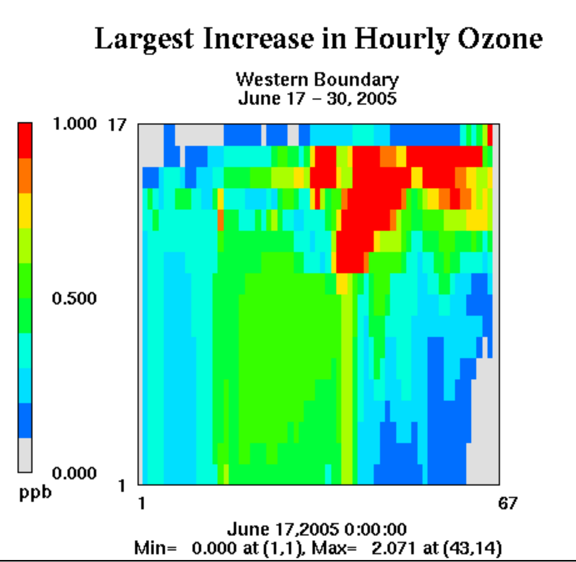
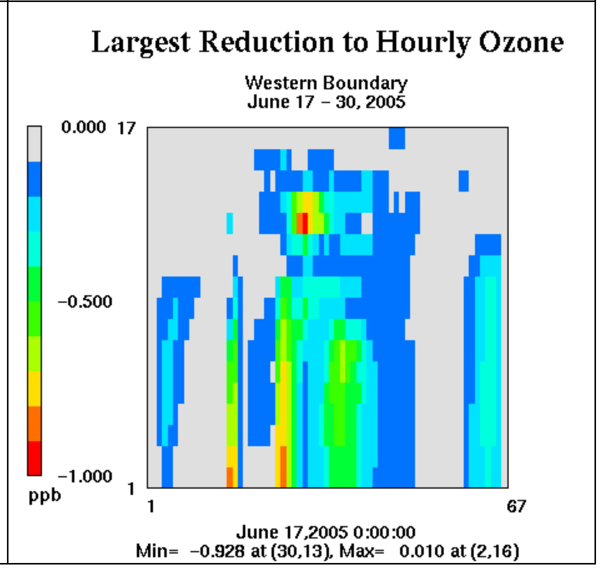
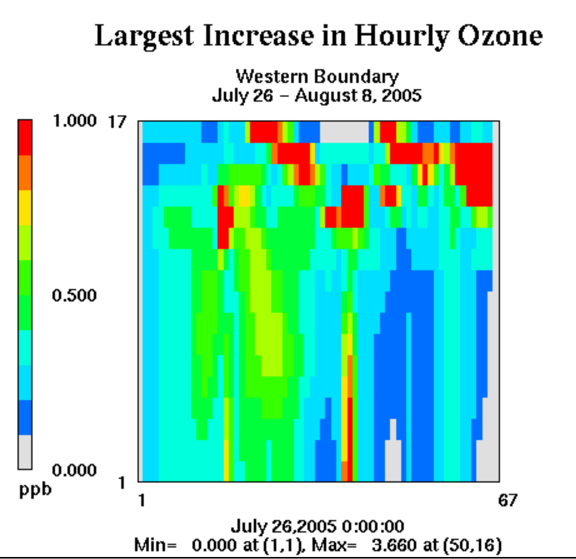
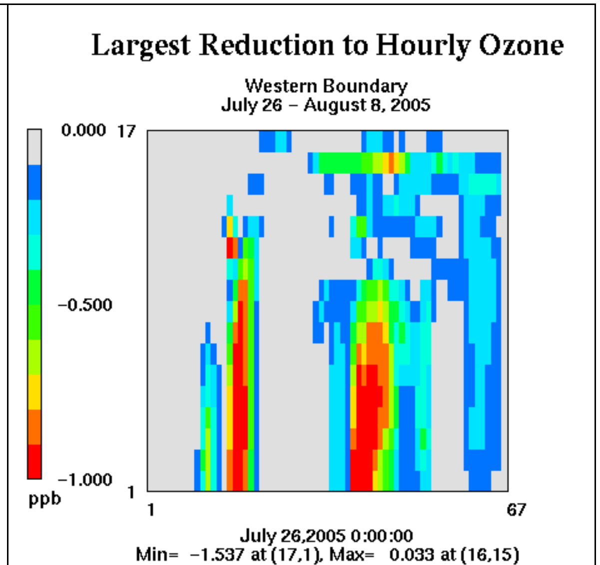
May 19-June 3, 2005 Max = 1.0 ppb Min = -1.1 ppb		
June 17 – 30, 2005 Max = 2.1 ppb Min = -0.9 ppb		

Figure 2-4. Vertical cross sections of the TCEQ western boundary showing the largest increases and decreases to hourly ozone in each episode between MOZART Run 1 and Run2.

July 26 – Aug 8, 2005

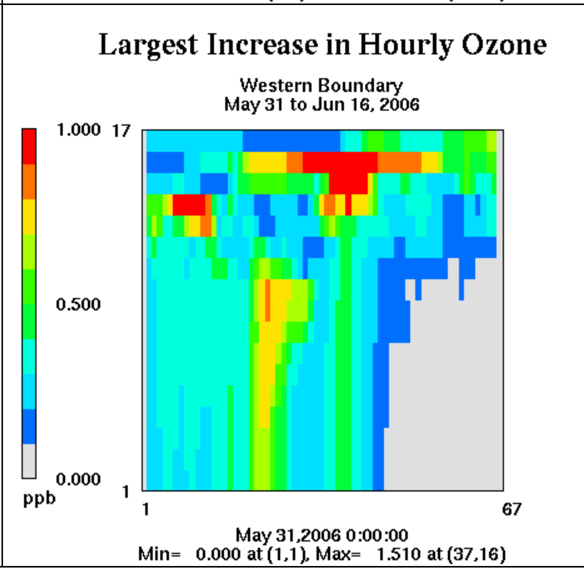
Max = 3.7 ppb
Min = -1.5 ppb





May 31 – June 16, 2006

Max = 1.5 ppb
Min = -1.9 ppb



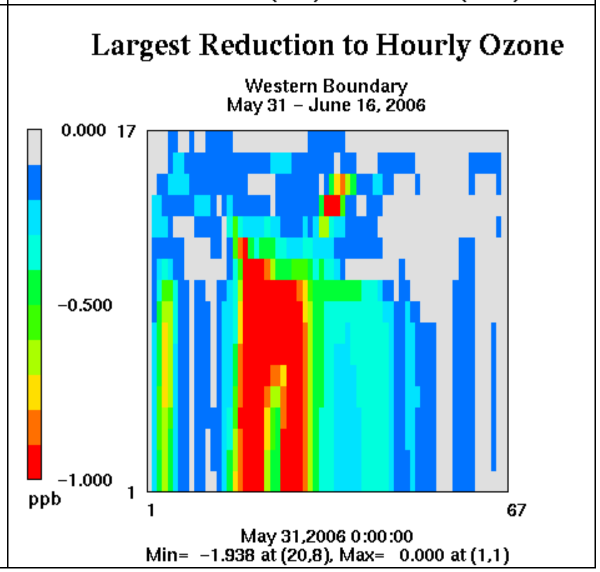


Figure 2-4 (continued). Vertical cross sections of the TCEQ western boundary showing the largest increases and decreases to hourly ozone in each episode between MOZART Run 1 and Run2.

Aug 1 – Oct 15, 2006

Max = 8.2 ppb
Min = -2.1 ppb

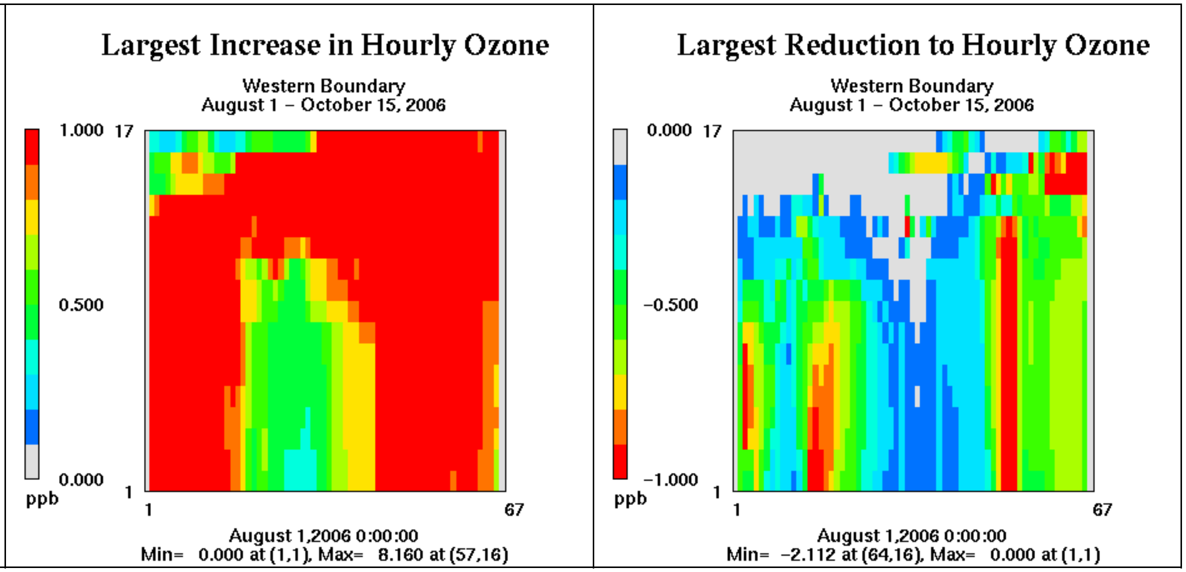


Figure 2-4 (concluded). Vertical cross sections of the TCEQ western boundary showing the largest increases and decreases to hourly ozone in each episode between MOZART Run 1 and Run2.

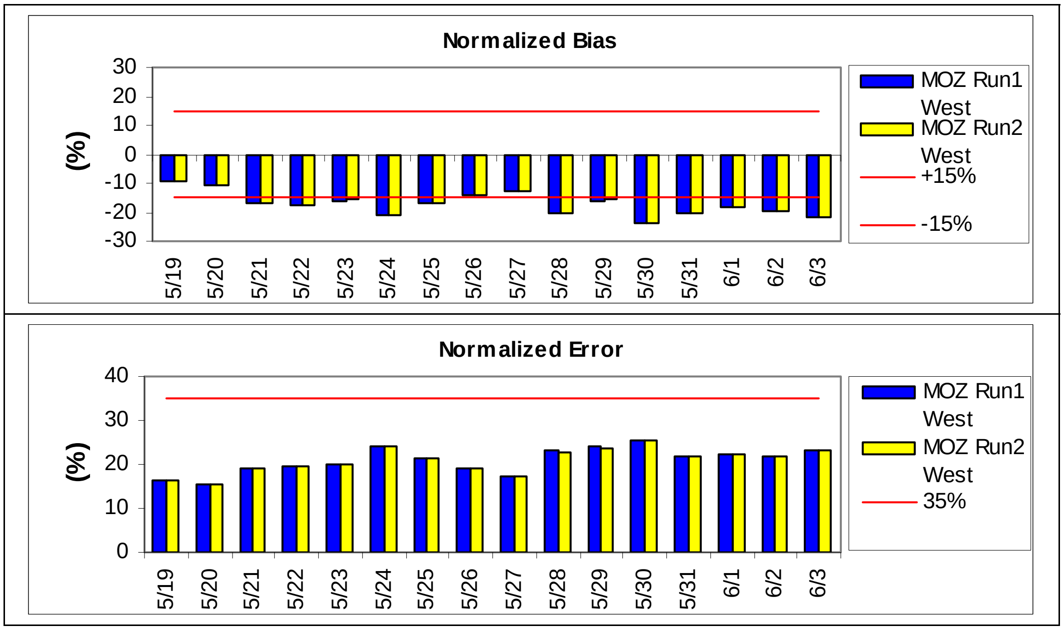


Figure 2-5. Normalized bias and error for 1 hour ozone at monitors near TCEQ's western boundary when using MOZART boundary conditions

<u>Updated GEOS-Chem Run</u>

The revised CAMx run using GEOS-Chem boundary conditions was identical to the first run performed in 2008 except for two changes – the boundary conditions and fire emissions. GEOS-Chem Run 2 incorporated 2005 and 2006 date-specific GEOS-Chem boundary conditions; Run 1 used 2002 monthly-averaged GEOS-Chem. The NCAR fire emissions processing was found to have little impact on the TCEQ boundaries, based on sensitivity tests using MOZART boundary conditions. Therefore, all differences between the two GEOS-Chem runs are assumed to result from the different boundary conditions.

Figure 2-6 shows the layer 1 average ozone from the CAMx run with date-specific GEOS-Chem at the TCEQ 36 km lateral boundaries using only the 44 dates that comprise the three 2005 episodes and the 93 episode dates in 2006 on the top left and right plots, respectively. Differences from GEOS-Chem Run 1 are shown in the bottom row.

In both base years, the highest average ozone in layer 1 was off the coast of New England on the TCEQ eastern boundary. GEOS-Chem Run 2 generated higher ozone than Run 1 throughout layer 1. In 2005, the largest increase was 5 ppb in the eastern boundary; in 2006, the northern boundary showed the greatest increase of over 7 ppb.

Figures 2-7 and 2-8 show time series of the daily averaged observed and predicted ozone between the two CAMx runs using GEOS-Chem boundary conditions during the summers of 2005 and 2006, respectively. The top three plots show the averages from all

AQS sites near the TCEQ western, southern, and northern boundaries. The bottom plot displays differences between the two GEOS-Chem boundary conditions.

The CAMx run using date-specific GEOS-Chem (Run2) predicted more ozone at surface sites near each of the three TCEQ boundaries on most dates, especially near the western boundary. GEOS-Chem Run 2 benefited sites near the western boundary the most because ozone was under predicted when using GEOS-Chem Run 1 on most dates.

In the southern boundary, both runs performed well during the first few weeks of May in both years; for the rest of the summer, ozone was well over predicted in both runs. Run 2 generally predicted more ozone than Run 1, but differences between the two runs were small compared to those in the western and northern boundaries.

Both GEOS-Chem runs over predicted ozone near the northern boundary on most dates. Run 2 predicted more ozone than Run 1.

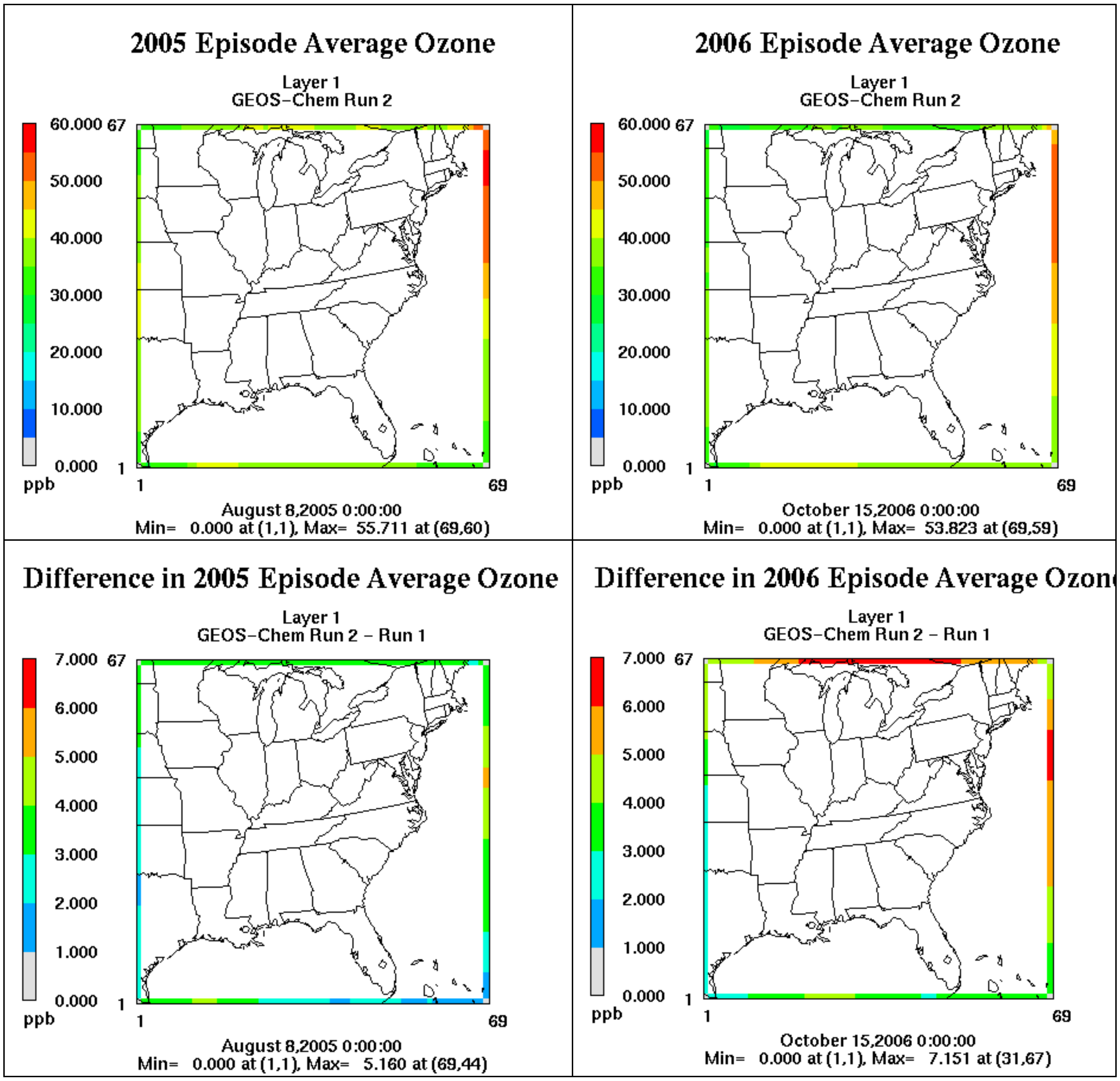


Figure 2-6. 2005 and 2006 episode averaged ozone in layer 1 when using date-specific GEOS-Chem and their differences when using 2002 monthly-averaged GEOS-Chem.

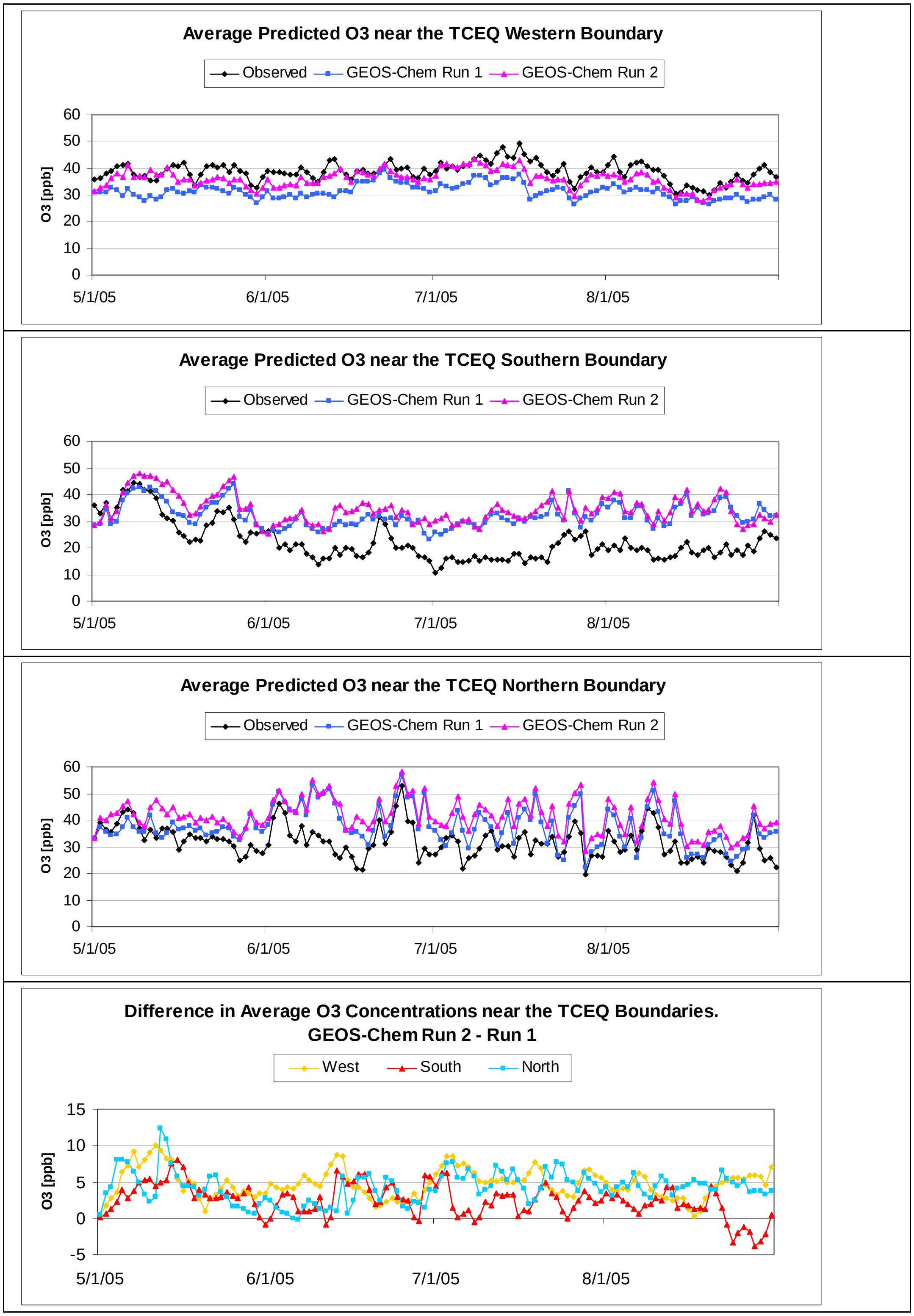


Figure 2-7. Time series of 2005 predicted and observed daily-average ozone near the TCEQ western, southern, and northern boundaries comparing CAMx Run 1 and Run 2 with GEOS-Chem. Differences are shown in the bottom-most plot.

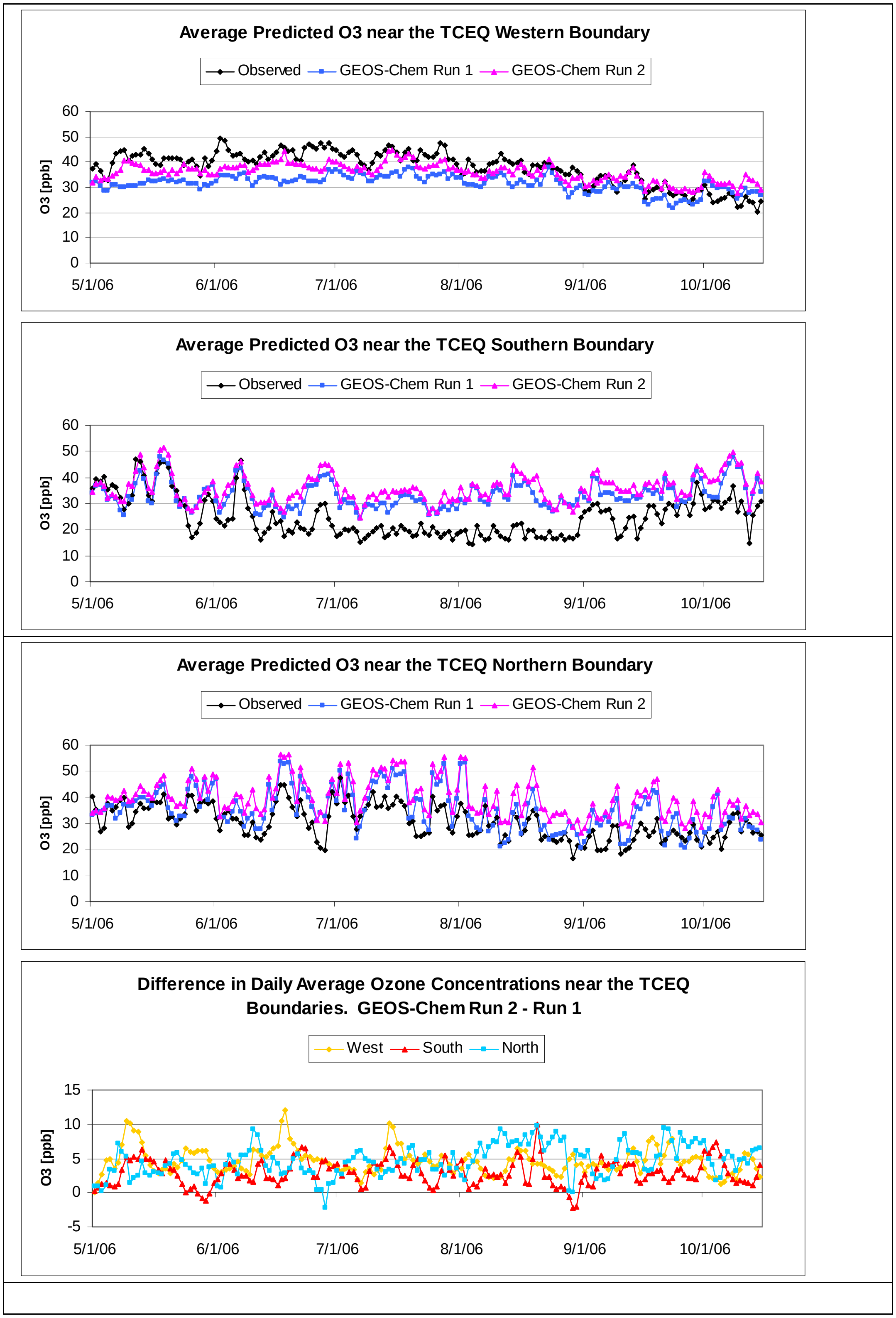


Figure 2-8. Time series of 2006 predicted and observed daily-average ozone near the TCEQ western, southern, and northern boundaries comparing CAMx Run 1 and Run 2 with GEOS-Chem. Differences are shown in the bottom-most plot.

Above the first layer, ozone was also higher in all lateral boundaries in Run 2 compared to Run 1. Figures 2-9 and 2-10 show vertical cross sections of the Run 2 time-averaged ozone in each of the four TCEQ lateral boundaries using only the episodic dates in 2005 and 2006, respectively. For the northern and southern boundary cross sections, the x-axis runs from west to east. For the western and eastern boundaries, the x-axis runs from south to north.

Ozone generally increased with height with average values in the lower 60s ppb in the top layer of each lateral boundary, except the 2006 southern boundary, where the highest average concentration was only 54 ppb. Top layer ozone tended to be low because the high levels of stratospheric ozone found in GEOS-Chem and MOZART were removed.

Figure 2-11 shows episode-averaged differences in ozone concentrations when using 2005 and 2006 date-specific GEOS-Chem derived boundary conditions (Run 2) compared to the GEOS-Chem 2002 monthly averages (Run 1). Vertical cross-sections across the TCEQ western, southern, and northern boundaries are displayed from left to right for each of the five episodes.

Date-specific GEOS-Chem increased the average ozone concentrations in all lateral boundaries and in all episodes, especially near the top of the domain. The only exception was in the July/August 2005 episode, when small ozone reductions were found in the southern boundary. The top of the northern boundary showed the largest increase in each of the five episodes, averaging as much as 18 ppb higher compared to the CAMx run using 2002 GEOS-Chem.

Since no observations were available to verify whether the higher ozone in Run 2 was better than Run 1, model performance at ozone monitoring sites near the ground will be assumed to be representative of the entire vertical column of each boundary.

Figure 2-12 shows bar charts of normalized bias and error for 1-hour ozone for each episode date in the May 19 to June 3, 2005 episode at sites near the TCEQ western, southern, and northern boundaries. CAMx with GEOS-Chem Run 2 predicted more ozone than Run 1 at monitoring sites near all three lateral boundaries, indicated by more positive (or less negative) normalized biases.

Run 2 benefited the western boundary the most. In Run 1, the normalized bias was negative and exceeded the ±15% performance goal on each date. Run 2 reduced the negative bias on all dates, meeting the performance goal for normalized bias on half of the 16 episode dates. The normalized bias averaged over all episode dates increased 9 percentage points, up from –24 % in Run 1 to –15 % in Run 2. Normalized error near the western boundary also improved on all dates, averaging 6 % lower.

Near the southern boundary, model performance was mixed. Since Run 2 tended to predict more ozone than Run 1, statistics favored Run 2 on dates when the normalized bias was negative and Run 1 on dates when the bias was positive.

In the TCEQ northern boundary, Run 1 performed better in the May, 2005 episode. Normalized bias was positive on most dates in Run 1, and more positive in Run 2.

Bar chart statistics for the other four episodes can be found in Appendix B. In all episodes, the date-specific 2005 and 2006 GEOS-Chem boundary conditions (Run 2) increased surface ozone near all three TCEQ lateral boundaries compared to Run 1. Run 2 consistently benefited the western boundary during most episode dates as normalized bias became less negative and normalized error was reduced on most dates.

Model performance tended to worsen near the southern boundary when using GEOS-Chem Run 2 since a majority of the episode dates had a positive bias in Run 1. Results were mixed in the northern boundary.

Overall, the consistent and much stronger performance at the western boundary suggests that the run using date-specific GEOS-Chem is advantageous over the run using 2002 monthly averaged GEOS-Chem.

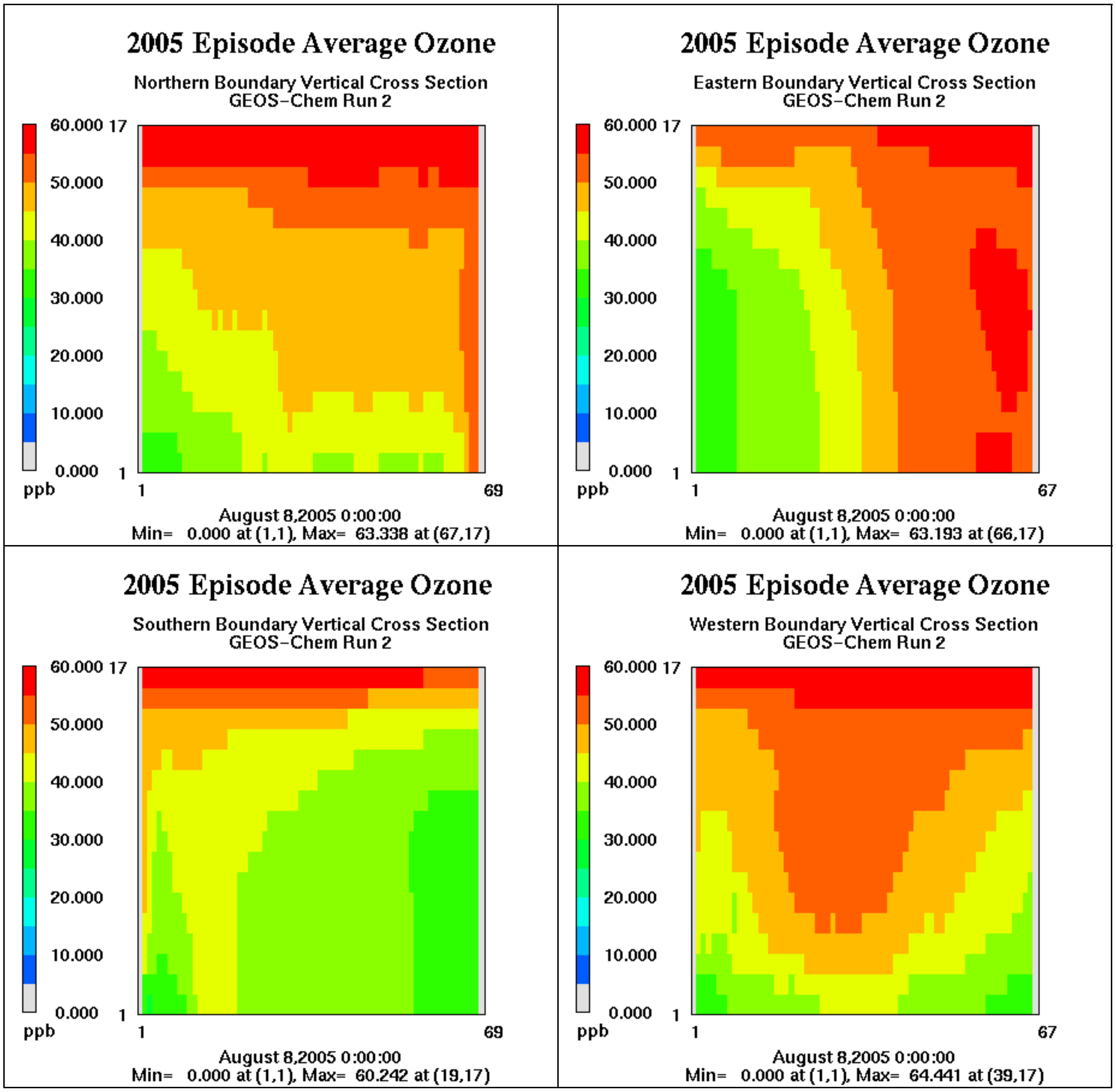


Figure 2-9. Vertical cross sections of the average 2005 ozone across the four TCEQ lateral boundaries when using date-specific GEOS-Chem.

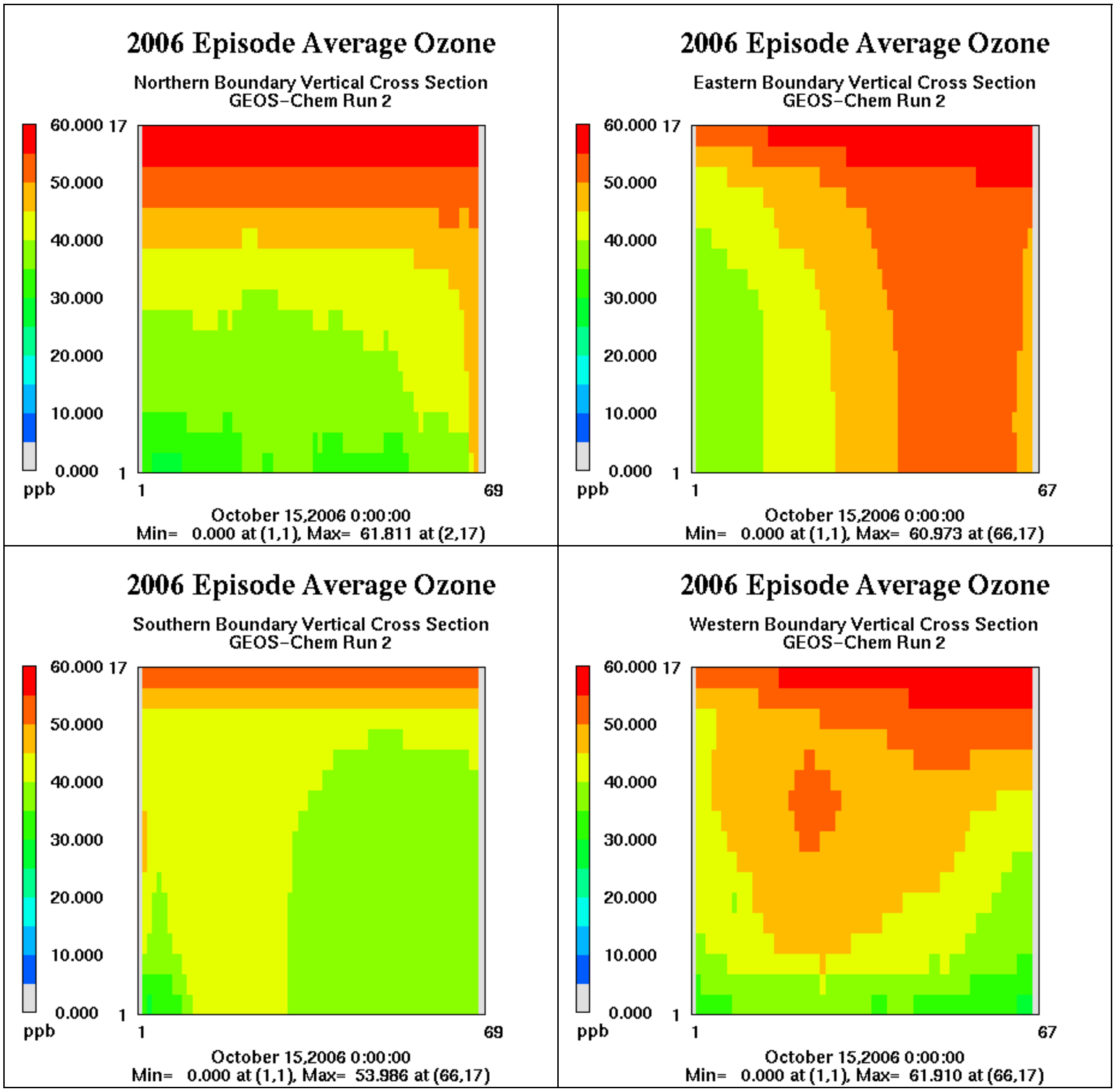


Figure 2-10. Vertical cross sections of the average 2006 ozone across the four TCEQ lateral boundaries when using date-specific GEOS-Chem.

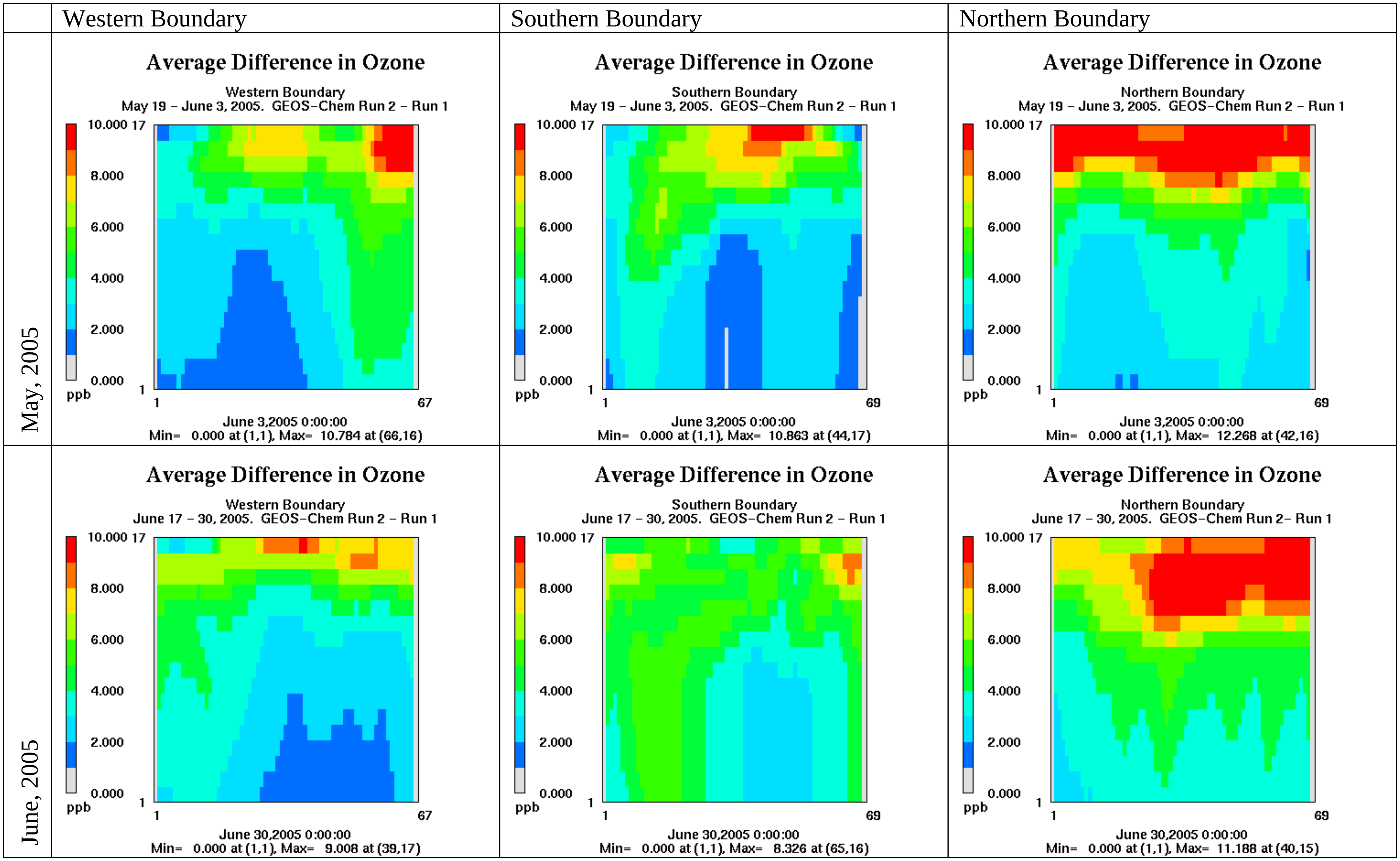


Figure 2-11. Differences in episode averaged ozone between GEOS-Chem Run 1 and Run 2 in vertical cross sections of the TCEQ western, southern, and northern boundaries

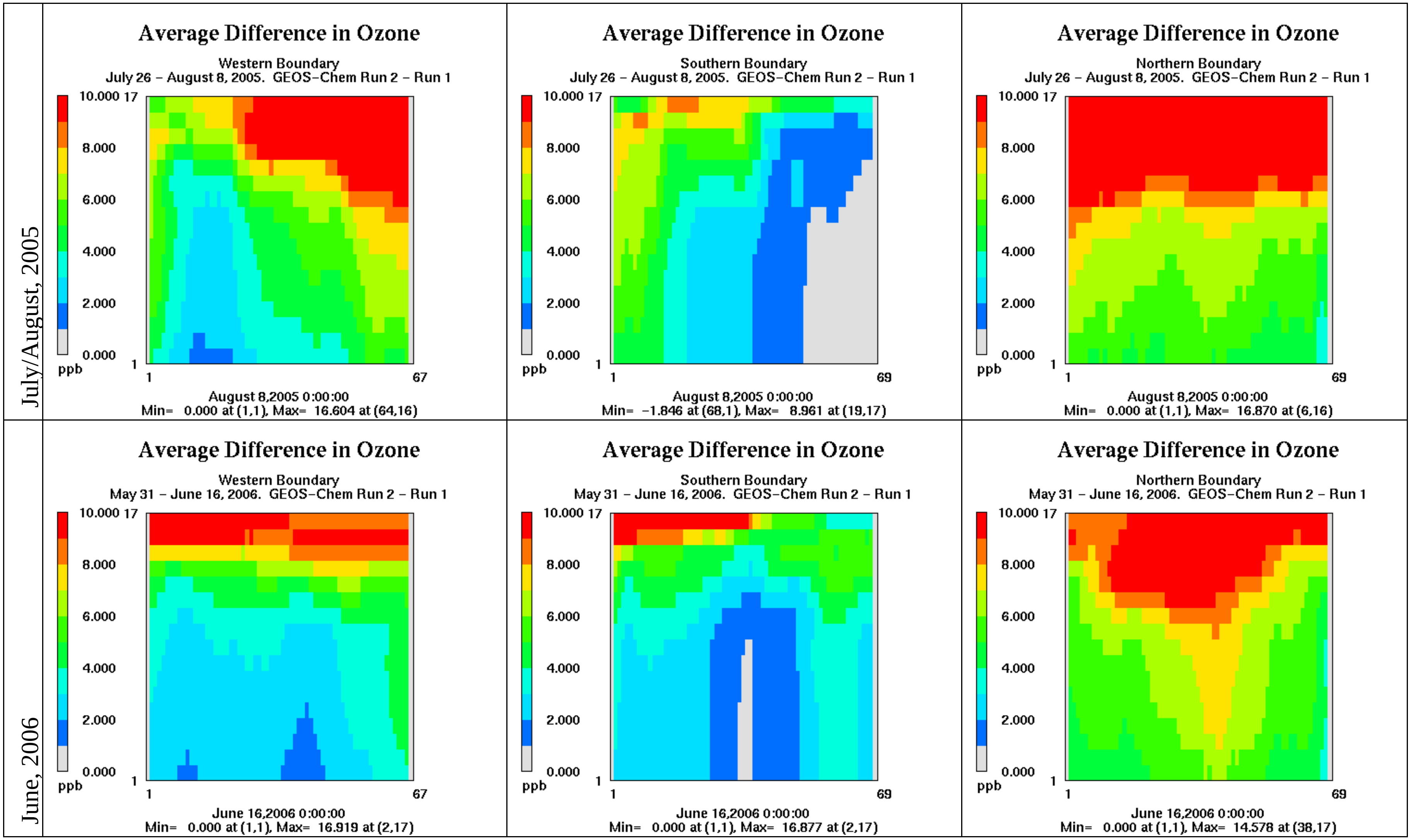


Figure 2-11 (continued). Differences in episode averaged ozone between GEOS-Chem Run 1 and Run 2 in vertical cross sections of the TCEQ western, southern, and northern boundaries

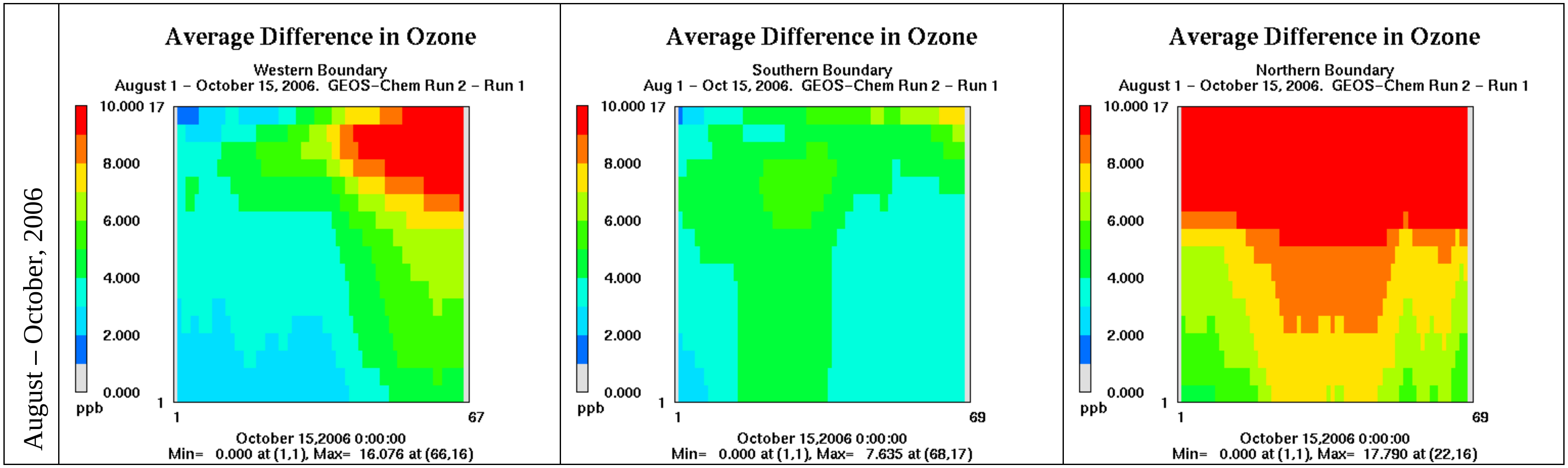


Figure 2-11 (concluded). Differences in episode averaged ozone between GEOS-Chem Run 1 and Run 2 in vertical cross sections of the TCEQ western, southern, and northern boundaries.

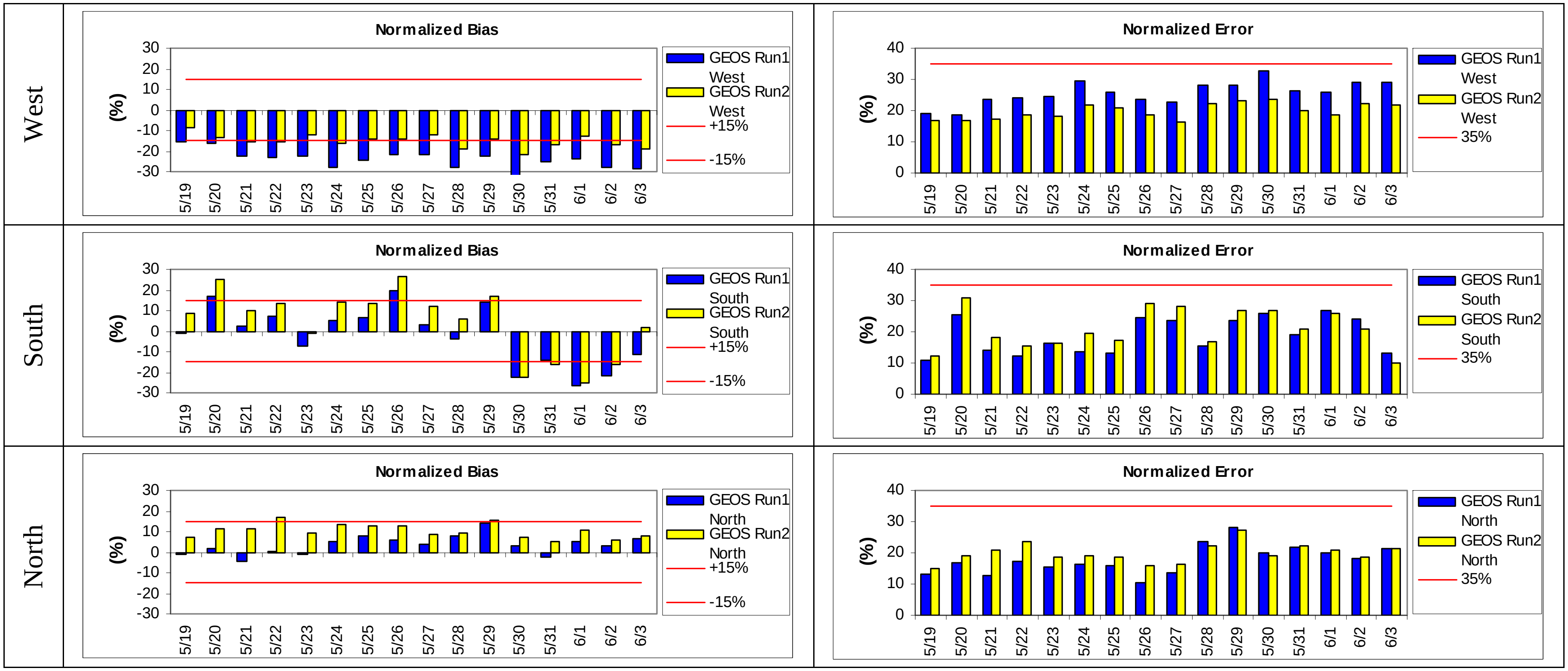


Figure 2-12. Normalized bias and error for the two runs with GEOS-Chem for 1-hour ozone at monitors near TCEQ's western, southern, and northern boundaries during the May 19 – June 3, 2005 episode.

MOZART Run 2 vs. GEOS-Chem Run 2

Comparisons were made between the CAMx run with date-specific MOZART and CAMx with date-specific GEOS-Chem. Figure 2-13 gives a quick perspective on how much ozone MOZART contributes in relation to the two GEOS-Chem runs. The figure shows time series of hourly ozone contributions from the RPO lateral boundaries to a grid cell over Houston using the inert mode in CAMx, in which emissions and chemistry are turned off. Date-specific GEOS-Chem (Run 2) always contributed more than 2002 monthly-averaged GEOS-Chem (Run 1); MOZART contributions tended to fall in between the two GEOS-Chem runs. The figure also shows that lateral boundaries always contribute more to Houston than the top boundary. These findings are representative of all five Houston episodes; similar plots for all episode dates can be found in Appendix C.

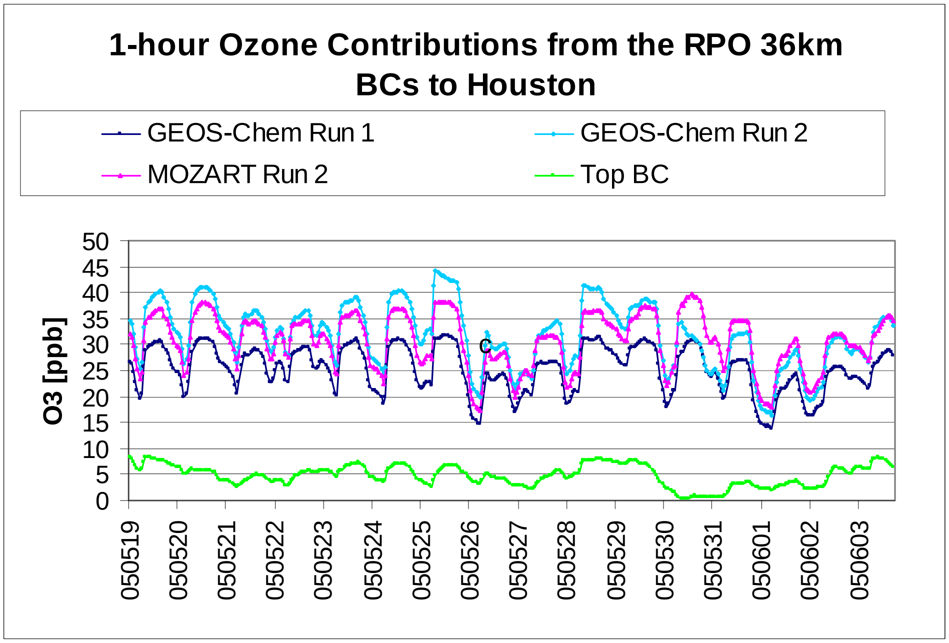


Figure 2-13. Time series of inert ozone contributions from the RPO 36 km lateral boundaries to Houston in the May, 2005 episode.

Figures 2-14 to 2-18 compare daily bar chart statistics for 1-hour ozone in the CAMx runs with date-specific MOZART and GEOS-Chem for each of the five Houston episodes. MOZART are in yellow; GEOS-Chem, blue. Each figure shows normalized bias and error on the left and right columns. Statistics are computed for the AQS ozone monitoring sites near the TCEQ western, southern, and northern boundaries shown from top to bottom. The red lines represent desired performance goals of ±15 % for normalized bias and 35 % for normalized error.

May 19 – June 3, 2005 Episode

In the TCEQ western boundary, normalized bias was negative on all dates from both runs. GEOS-Chem Run 2 performed slightly better than MOZART on most dates in the western boundary as normalized bias became less negative and normalized error was reduced.

Differences in model performance statistics were much smaller than the differences between the two GEOS-Chem runs.

In the northern boundary, GEOS-Chem Run 2 performed much better than MOZART as the positive bias on all dates was reduced with GEOS-Chem Run 2. MOZART had 7 episodes dates with a normalized bias exceeding 15 %; GEOS-Chem had only 1 exceedance date. In the southern boundary, performance was mixed with large differences in statistics during the last few days of the episode.

Overall, date-specific GEOS-Chem performed better than MOZART in the May, 2005 episode.

June 17 – 30, 2005 Episode

In the June, 2005 episode, CAMx with GEOS-Chem Run 2 predicted more surface ozone near all three TCEQ boundaries on all dates compared to MOZART. In the western TCEQ boundary, where normalized bias was negative on all dates in both runs, GEOS-Chem Run 2 performed much better than MOZART. All dates met the ±15 % performance goal for normalized bias when using date-specific GEOS-Chem; MOZART only met this goal on 5 of the 14 dates.

In the northern and southern boundaries, MOZART performed better. Since most dates had a positive bias with MOZART, the higher ozone when using date-specific GEOS-Chem increased the bias and error even higher. Even though model performance suffered when using date-specific GEOS-Chem, most dates in the northern boundary remained within the ± 15 % performance goal.

July 26 – August 8, 2005 Episode

In the July/August, 2005 episode, normalized bias was higher on all dates and in all three lateral boundaries when using date-specific GEOS-Chem compared to MOZART. In the western boundary, where normalized biases were negative on all dates in both runs, GEOS-Chem produced less negative biases and lower errors than MOZART on all episode dates. The number of dates exceeding the ± 15% normalized bias goal was reduced from 13 when using MOZART to 2 when using date-specific GEOS-Chem. GEOs-Chem Run 2 performance was worse in the southern boundary and mixed in the north.

May 31 – June 16, 2006 Episode

In the June, 2006 episode, GEOS-Chem continued to show more positive (or less negative) normalized biases compared to MOZART in all three lateral boundaries on most dates. Near the TCEQ western boundary, model performance was better when using date-specific GEOS-Chem on all episode dates as more surface ozone was predicted. Near the southern TCEQ boundary, MOZART had a positive bias on most dates and was even higher with GEOS-Chem Run 2. Performance was mixed in the northern boundary.

August 1 – October 15, 2006 Episode

The August to October, 2006 episode was evaluated in three monthly intervals. In August, the greater ozone predicted when using date-specific GEOS-Chem favored GEOS-Chem in the western boundary, where the normalized bias was negative on all dates, and favored MOZART in the southern boundary, where the normalized bias was positive on all dates. Performance was mixed in the northern boundary.

In September, 2006, both date-specific GEOS-Chem and MOZART performed well near the western boundary as most dates were within the ±15 % goal for normalized bias and 35 % for normalized error. Date-specific GEOS-Chem continued to perform better near the TCEQ western boundary. In the southern boundary, MOZART did not show a distinctive advantage over GEOS-Chem. Like other episode dates, GEOS-Chem predicted more ozone than MOZART. Unlike other episode periods, more dates showed negative biases when using MOZART; therefore, performance improved on these dates when GEOS-Chem introduced higher ozone. Performance in the northern boundary was mixed.

October, 2006 was the only month in which the normalized bias was positive near the western boundary on a majority of dates when using MOZART. Unlike all other episode dates, normalized bias was less positive on most dates in the western boundary when using date-specific GEOS-Chem. GEOS-Chem also performed better in the northern boundary due to its performance on October 13 and 14, when MOZART's normalized bias and error were much higher than GEOS-Chem. Performance near the TCEQ southern boundary was mixed.

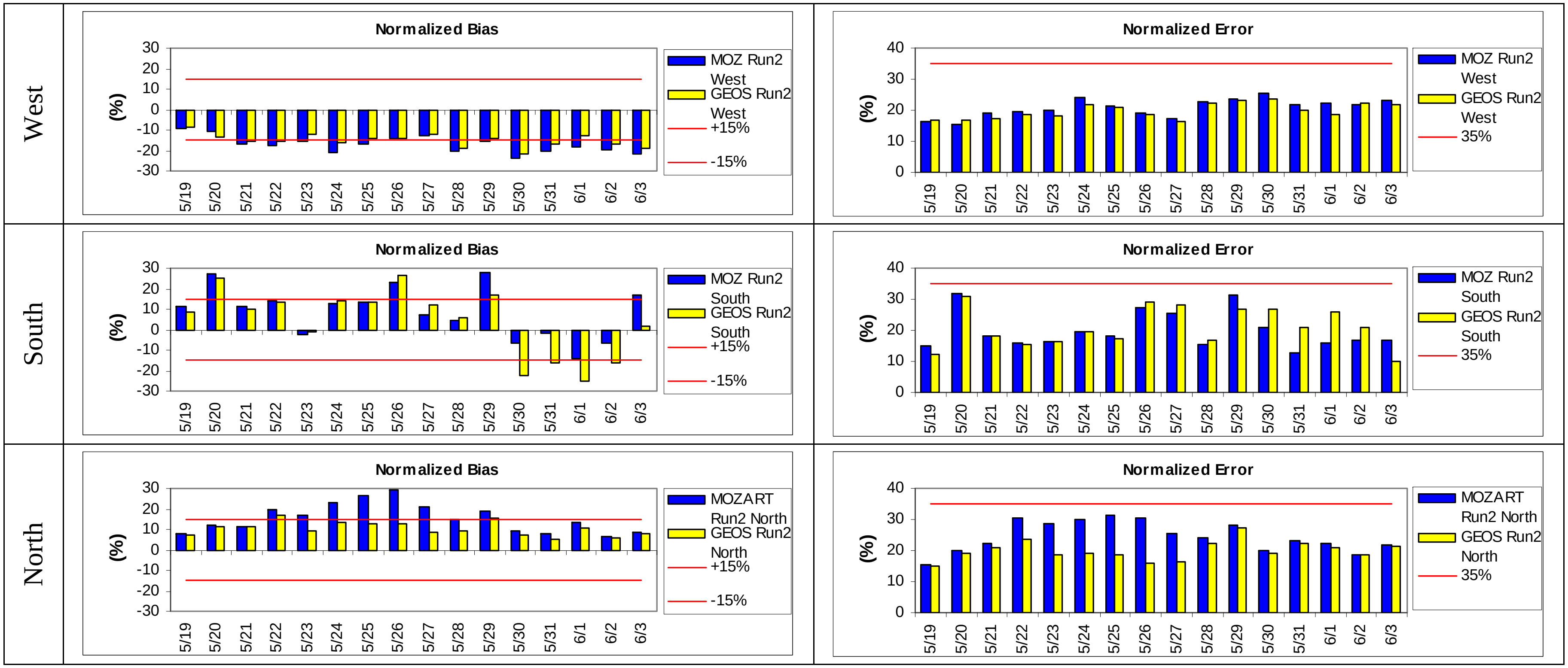


Figure 2-14. Normalized bias and error comparing MOZART Run 2 to GEOS-Chem Run 2 for 1-hour ozone at monitors near TCEQ's western, southern, and northern boundaries during the May, 2005 episode.

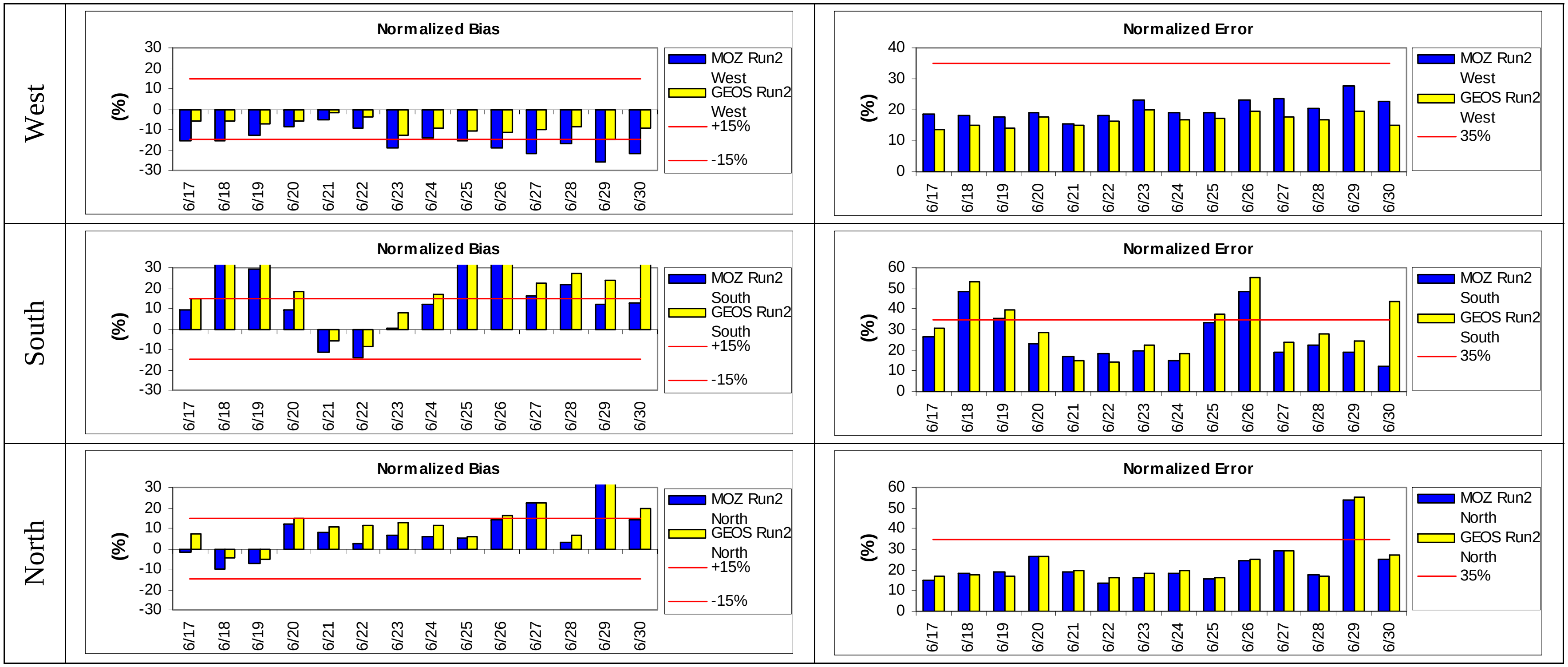


Figure 2-15. Normalized bias and error comparing MOZART Run 2 to GEOS-Chem Run 2 for 1-hour ozone at monitors near TCEQ's western, southern, and northern boundaries during the June, 2005 episode.

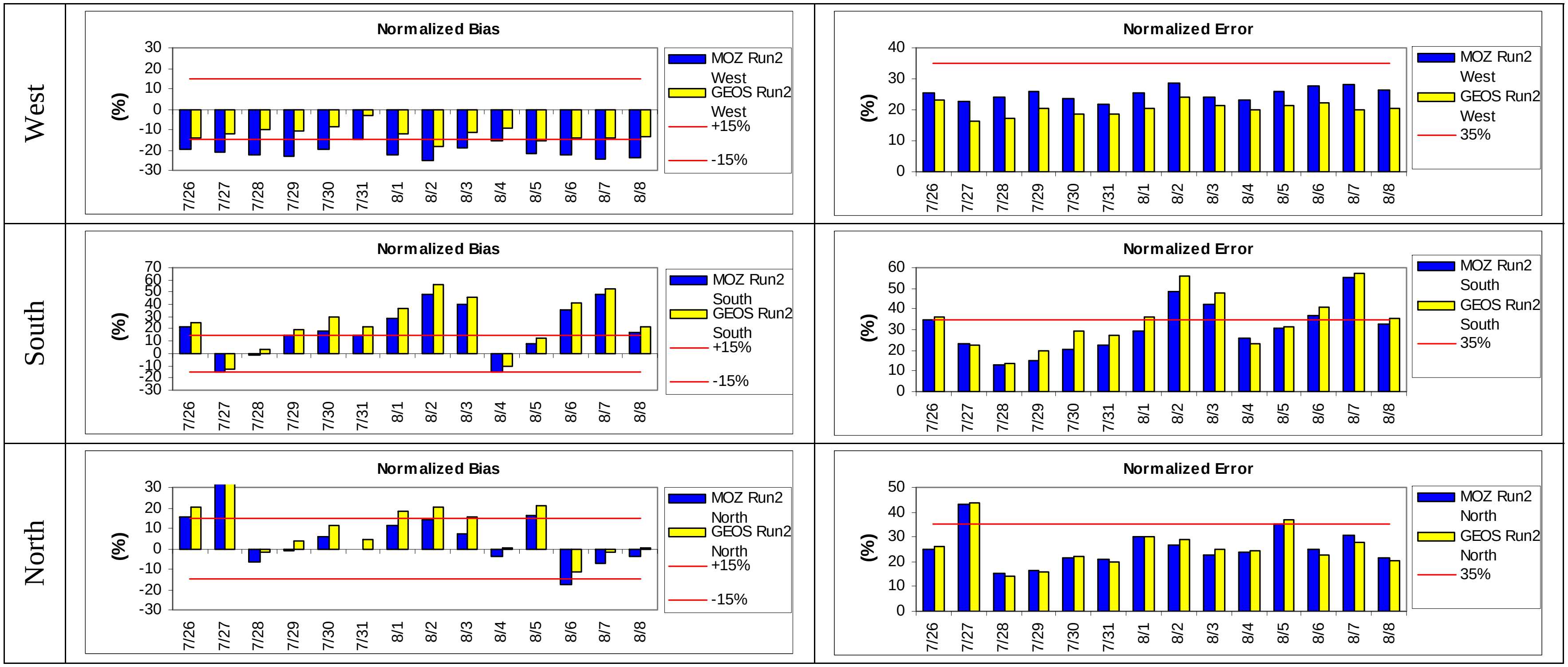


Figure 2-16. Normalized bias and error comparing MOZART Run 2 to GEOS-Chem Run 2 for 1-hour ozone at monitors near TCEQ's western, southern, and northern boundaries during the July/August, 2005 episode.

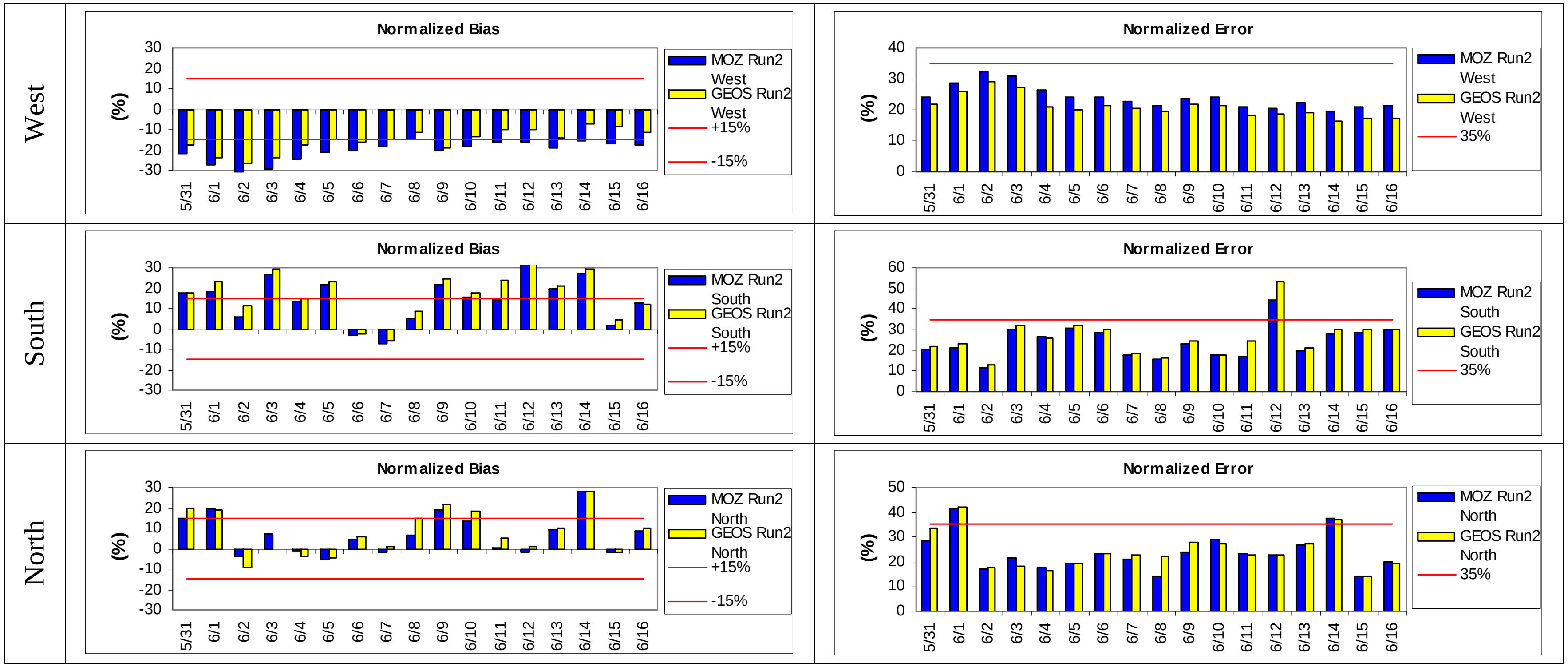


Figure 2-17. Normalized bias and error comparing MOZART Run 2 to GEOS-Chem Run 2 for 1-hour ozone at monitors near TCEQ's western, southern, and northern boundaries during the June, 2006 episode.

Figure 2-18. Normalized bias and error comparing MOZART Run 2 to GEOS-Chem Run 2 for 1-hour ozone at monitors near TCEQ's western, southern, and northern boundaries during the August to October, 2006 episode.

Figure 2-18 (continued). Normalized bias and error comparing MOZART Run 2 to GEOS-Chem Run 2 for 1-hour ozone at monitors near TCEQ's western, southern, and northern boundaries during the August to October, 2006 episode.

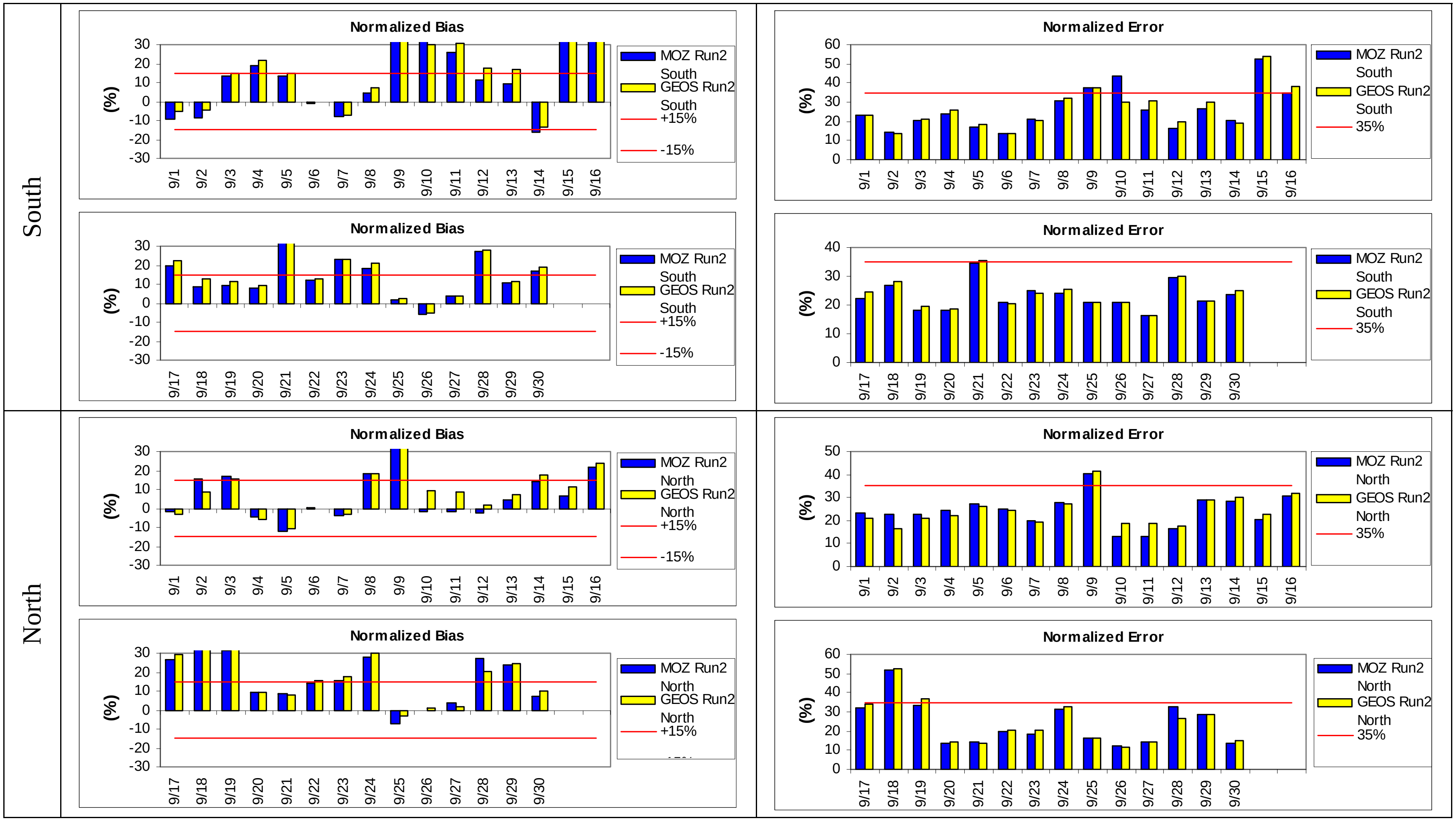


Figure 2-18 (continued). Normalized bias and error comparing MOZART Run 2 to GEOS-Chem Run 2 for 1-hour ozone at monitors near TCEQ's western, southern, and northern boundaries during the August to October, 2006 episode.

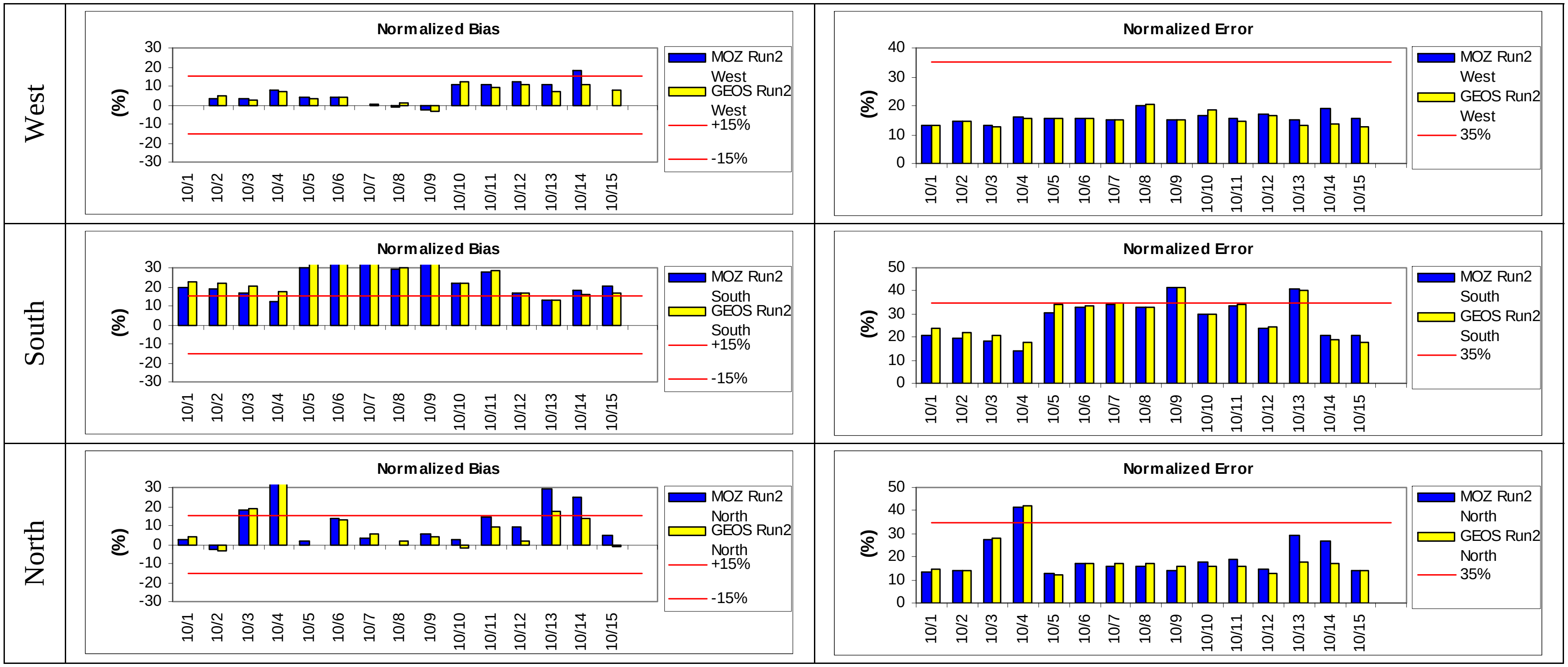


Figure 2-18 (concluded). Normalized bias and error comparing MOZART Run 2 to GEOS-Chem Run 2 for 1-hour ozone at monitors near TCEQ's western, southern, and northern boundaries during the August to October, 2006 episode.

2.3 SUMMARY

Among the five Houston episodes in 2005 and 2006, the use of date-specific GEOS-Chem generally resulted in more surface ozone near the TCEQ boundaries than date-specific MOZART, and even more ozone than the 2002 monthly averaged GEOS-Chem. In the western TCEQ boundary, ozone was under predicted on almost all episode dates in all runs. The higher ozone from date-specific GEOS-Chem improved normalized bias and error on almost every episode date. In the southern TCEQ boundary, where normalized bias tended to be positive on most episode dates, performance either favored MOZART or tended to be mixed. In the northern boundary, model performance tended to be mixed on most episode dates, but GEOS-Chem tended to perform better in the May, 2005 episode and during October, 2006.

Overall, mixed performance in the northern and southern TCEQ boundaries and consistent performance by date-specific GEOS-Chem in the western TCEQ boundary suggests that boundary conditions extracted from the CAMx RPO run with date-specific GEOS-Chem is recommended for further evaluation.

3.0 2018 FUTURE YEAR MODELING

CAMx 2018 future year modeling of the May 1 to September 1, 2005 and May 1 to October 16, 2006 periods was performed for the 36 km RPO domain in order to extract future year boundary conditions for the TCEQ domain. Inputs were identical to the base year runs, except for the emissions.

Future year emissions were based on the WRAP 2018 Preliminary Reasonable Progress (PRP18) inventory and typical fire emissions from the CENRAP Typical 02g inventory. The typical fire inventory consisted of point sources when the fire location and date were known; otherwise, the fire was treated as an area source. Point sources were updated to address the time zone shift in the PSTFIR module of EPS3, which handles the vertical allocation for each fire. In the 2005 and 2006 base years, the update to the NCAR satellite-based fire emissions were found to have very little impact near the TCEQ 36 km lateral boundaries. The same would be expected for the CENRAP typical fire inventory.

Two 2018 future year runs were performed using the same 2005 and 2006 date-specific biogenics and boundary conditions as were used in the base years. Date-specific 2018 GEOS-Chem and MOZART outputs were not available. The updated CAMx 2018 MOZART run (Run 2) was configured exactly like the original future year CAMx 2018 MOZART run performed in 2008 (Tai et al., 2008), but with corrected fire emissions. Ozone differences from the original future year MOZART run were small and will not be discussed further.

The second run updated both the typical fire emissions and replaced the 2002 monthly averaged GEOS-Chem boundary conditions with 2005 and 2006 date-specific GEOS-Chem.

3.1 MODEL RESULTS: 2018 VS. BASE YEAR

Figures 3-1 and 3-2 show time series of daily averaged ozone between the GEOS-Chem Run 2 base year and corresponding 2018 future year runs for the summers of 2005 and 2006, respectively. Each figure shows time series of daily averaged ozone at AQS sites near the TCEQ western, southern, and northern boundaries. Base year observed averages were added for reference purposes only. The plot on the bottom of each figure displays differences between 2018 and the corresponding base year for each lateral boundary.

Future year ozone near the TCEQ surface boundaries was generally lower than in the base year. The biggest change occurred in the northern boundary. In the 2005 base year, 2018 ozone in the northern boundary averaged a 4.5 ppb reduction; in the 2006 base year, future year ozone was reduced by 3.5 ppb. Reductions to 2018 ozone near the western and southern boundaries were smaller, averaging just over 1 ppb lower in the west and 0.2 ppb in the south for both base years.

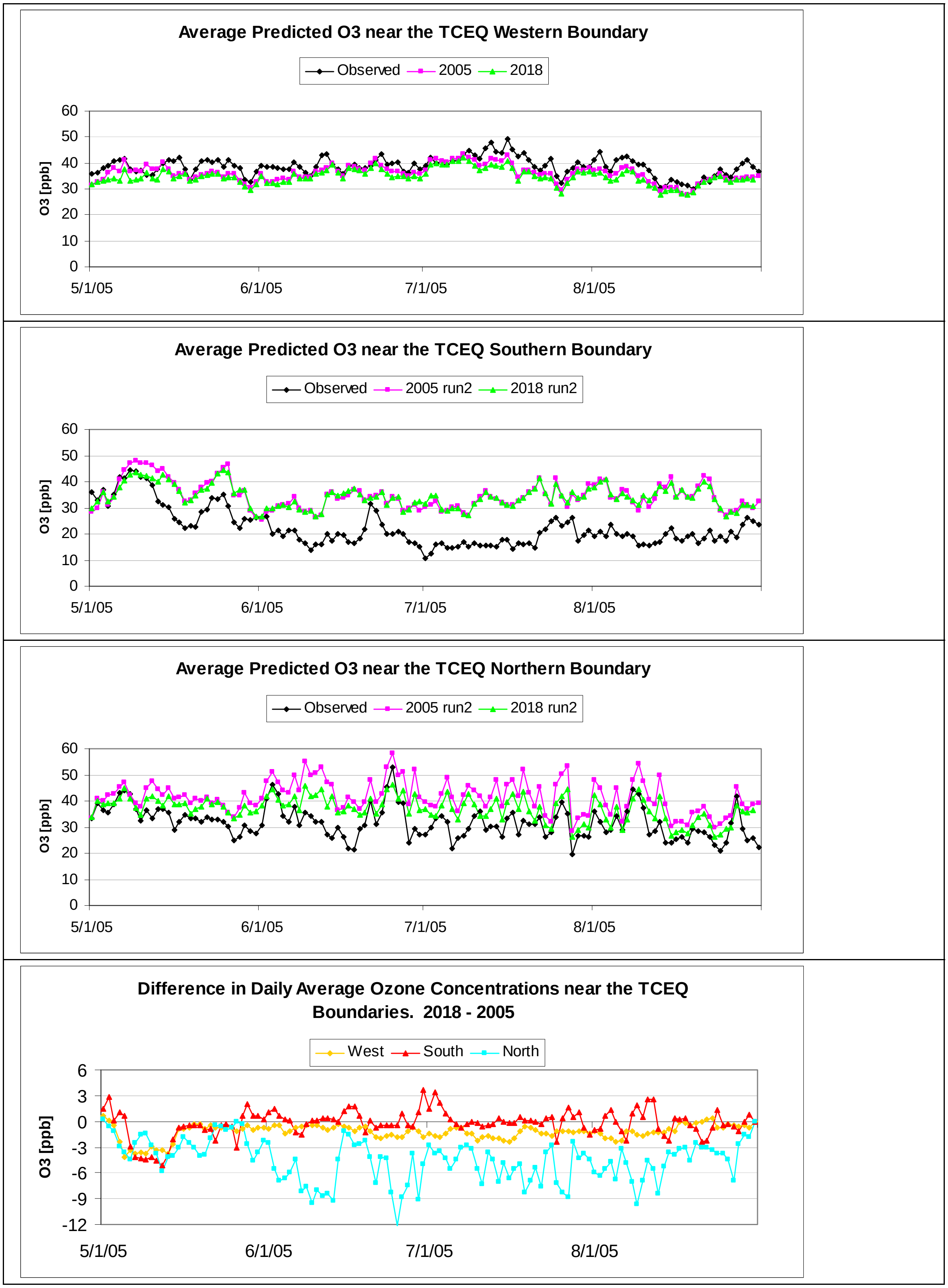


Figure 3-1. Time series of 2005 and corresponding 2018 daily averaged ozone near the TCEQ western, southern, and northern lateral boundaries using 2005 GEOS-Chem. Differences in each lateral boundary are shown in the bottom-most plot.

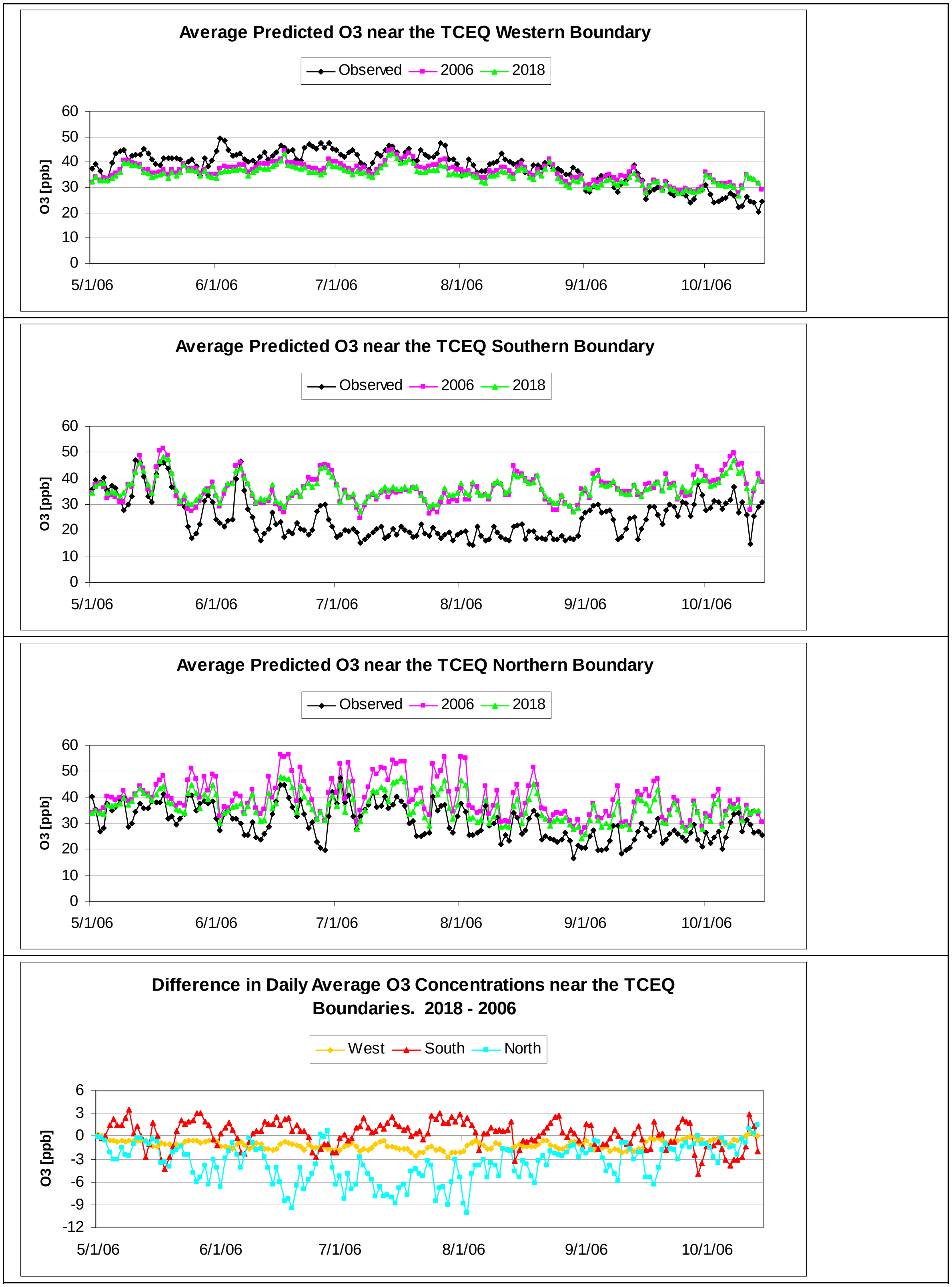


Figure 3-2. Time series of 2006 and corresponding 2018 daily averaged ozone near the TCEQ western, southern, and northern lateral boundaries using 2006 GEOS-Chem. Differences in each lateral boundary are shown in the bottom-most plot.

Aloft, the average future year boundary conditions were also lower in 2018 compared to the base year. Figure 3-3 displays vertical cross sections of the four TCEQ lateral boundaries, showing the change in average ozone during the 44 episode dates in 2005 from the base year to 2018. Ozone reduction was largest in the northeast, where future year ozone was up to 8 ppb lower, and smallest along the southern boundary.

Similar plots for the 2006 base year are shown in Figure 3-4. The average ozone reduction in 2018 was smaller compared to changes from 2005. TCEQ lateral boundaries near New England tended to show the greatest reductions in the future year; boundaries over the Gulf of Mexico showed the least change.

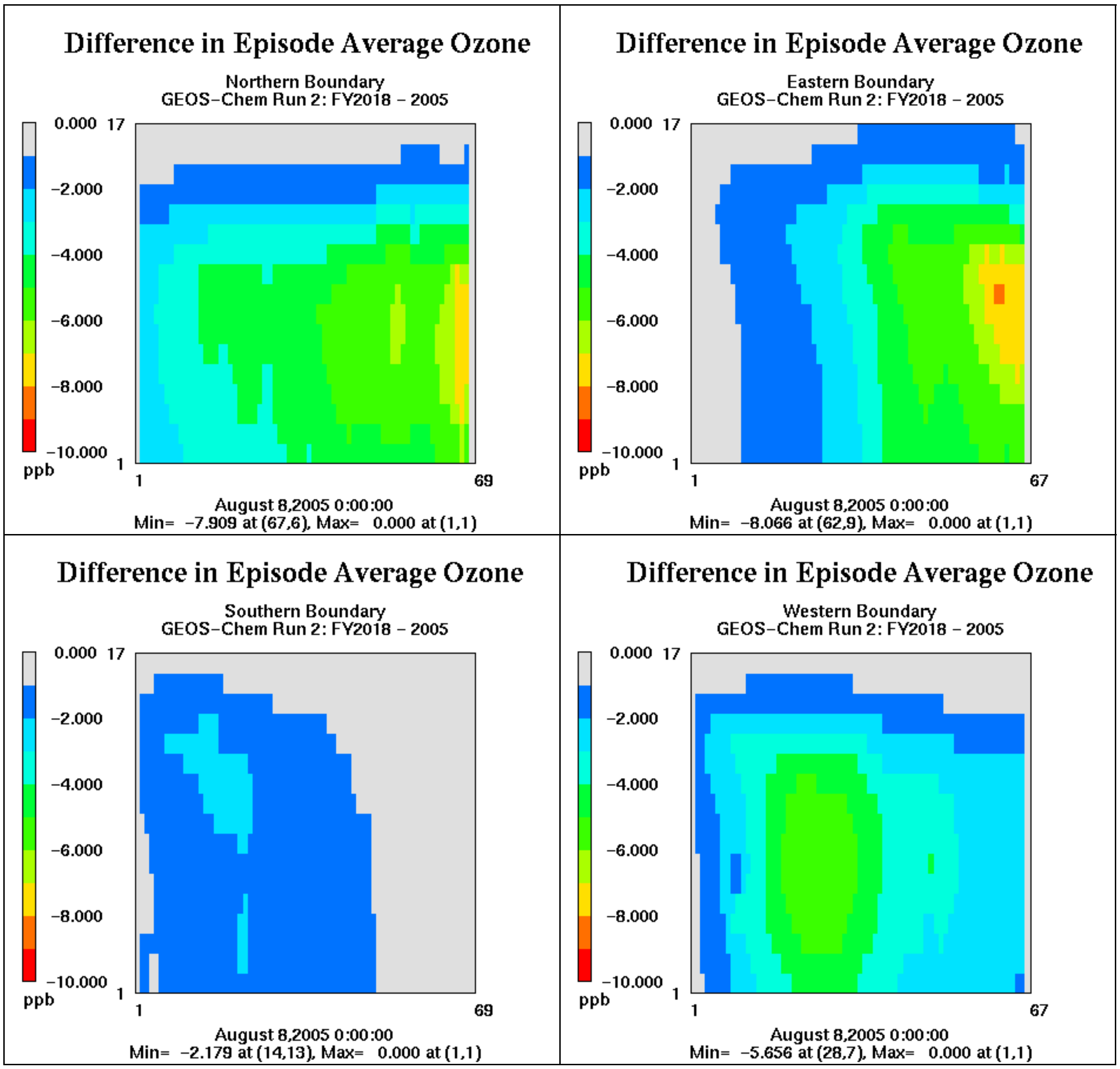


Figure 3-3. Vertical cross sections of ozone differences between 2005 and 2018 in each of the four TCEQ lateral boundaries when using 2005 GEOS-Chem

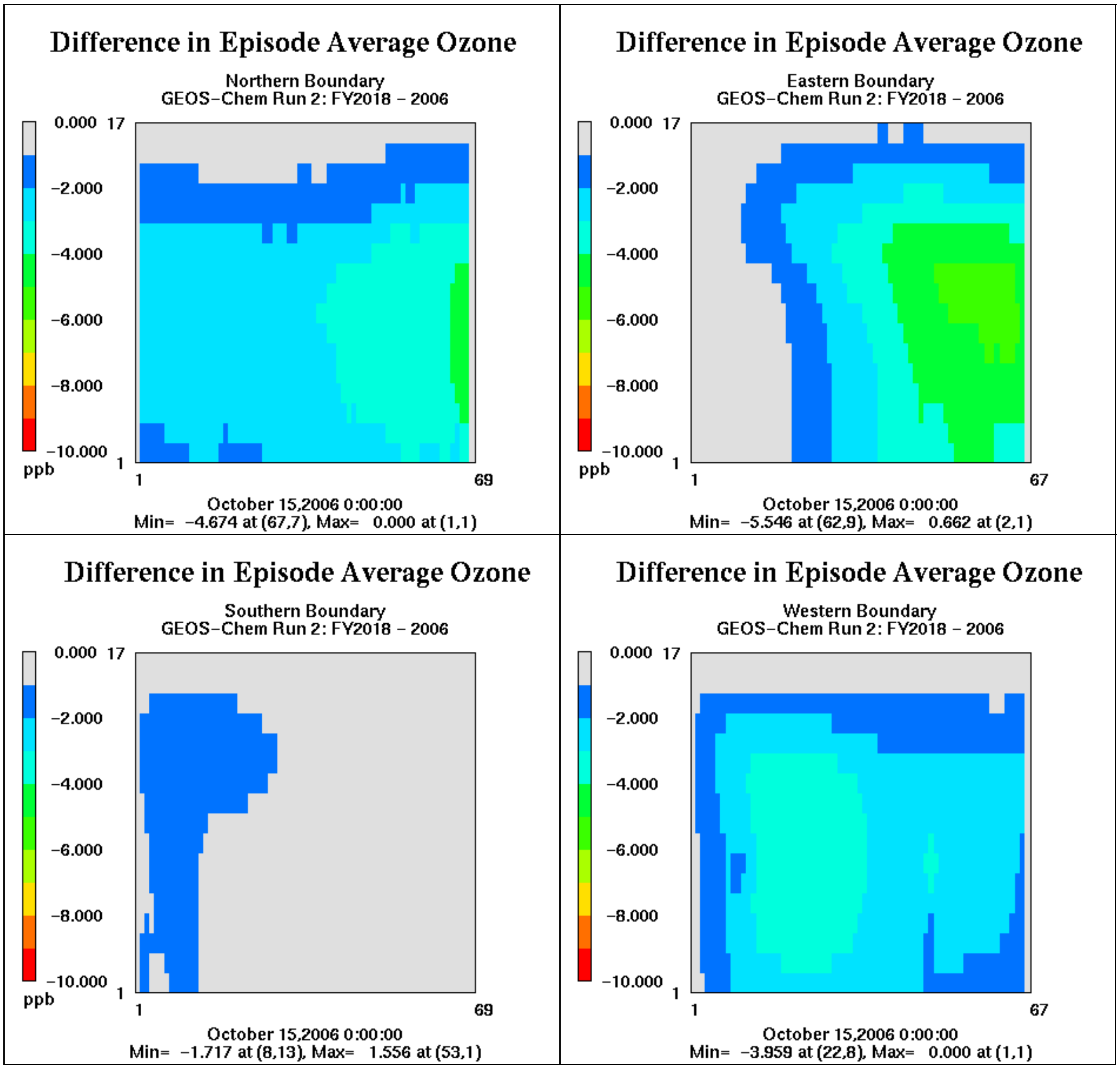


Figure 3-4. Vertical cross sections of ozone differences between 2006 and 2018 in each of the four TCEQ lateral boundaries when using 2006 GEOS-Chem

NCAR vs. CENRAP Typical Fire Emissions

One issue raised in the 2008 report was the large difference in emissions between the 2005 and 2006 date-specific fire emissions based on NCAR satellite data and the CENRAP typical fire emissions inventory. CAMx used NCAR fire emissions for the base years and typical fires for the 2018 future year. The typical fires consisted of point source emissions when the location and date of the fire was known; otherwise, fires were treated as area sources. Table 3-1 lists the total NOx, VOC, and CO fire emissions in the RPO domain on five random dates representing a Wednesday in each episode.

On May 25, 2005 and June 7, 2006, the NCAR fire emissions of NOX, VOC, and CO doubled the CENRAP typical fire emissions. On the other three dates, typical fire NOx emissions were at least 40 % larger than NCAR fire emissions. A CAMx sensitivity test was performed for the 2005 and 2006 base years. CENRAP typical fire emissions were incorporated into the base year emissions instead of the NCAR satellite fire inventory to evaluate the sensitivity to different fire emission inventories. MOZART boundary conditions were used in the sensitivity tests, and were compared to the MOZART run using NCAR fire emissions data.

Table 3-1. Typical vs. satellite-derived fire emissions in the RPO domain.

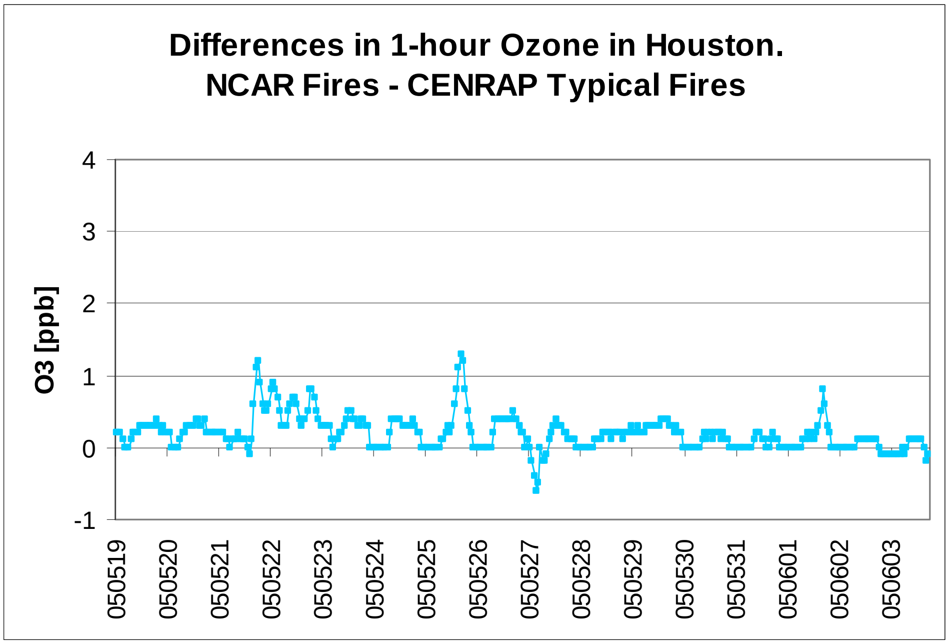
	NOx [tpd]		VOC [tpd]		CO [tpd]	
	NCAR	Typical	NCAR	Typical	NCAR	Typical
25-May-05	2252	1086	6746	2720	98200	50257
22-Jun-05	1692	2362	3462	5382	54200	108242
3-Aug-05	1127	2503	2454	5600	35900	114196
7-Jun-06	1228	591	2759	1644	41100	27258
23-Aug-06	6497	9181	13300	20262	211000	426033

Hourly ozone was extracted for a single cell over Houston to illustrate differences in hourly ozone when using NCAR fires instead of the CENRAP typical fire inventory. Time series showing differences in hourly ozone in Houston due to different fire inventories for each of the five episodes are shown in Figure 3-5 for all five episodes.

The use of NCAR fire emissions in the base year resulted in more ozone over Houston than the CENRAP typical fire inventory during most hours. In the May and June, 2005 episodes, the hourly differences were small with most changes under 1 ppb. In the July/August, 2005 episodes, differences during most hours were under 1 ppb, but two dates spiked higher when using NCAR satellite-derived fires – July 30 and August 7, when 1-hour ozone was 2 ppb and 5 ppb higher, respectively, when compared to the run using typical fires.

Differences were more pronounced in the 2006 episode. Ozone was up to 7 ppb higher on two dates when using NCAR fires instead of CENRAP fires – June 13 and October 5, 2006. There were 12 dates in the August-October, 2006 episode when the use of NCAR fires instead of CENRAP typical fires raised hourly ozone in Houston over 2 ppb.

The use of different fire emission inventories for ozone SIP modeling has the potential to affect the amount of controls needed. In the current situation, the use of NCAR fires in the base year and CENRAP typical fires in the future year would result in higher ozone in the base year and relatively less in the future year. This scenario would lead to lower relative reduction factors and potentially lower future design values. Caution may be needed when mixing the inventories.



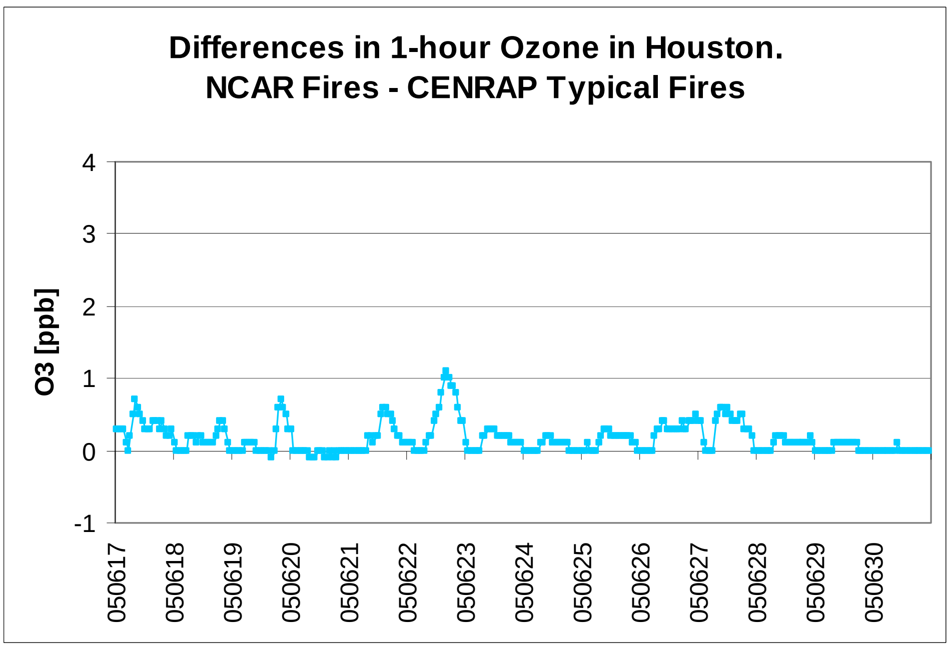
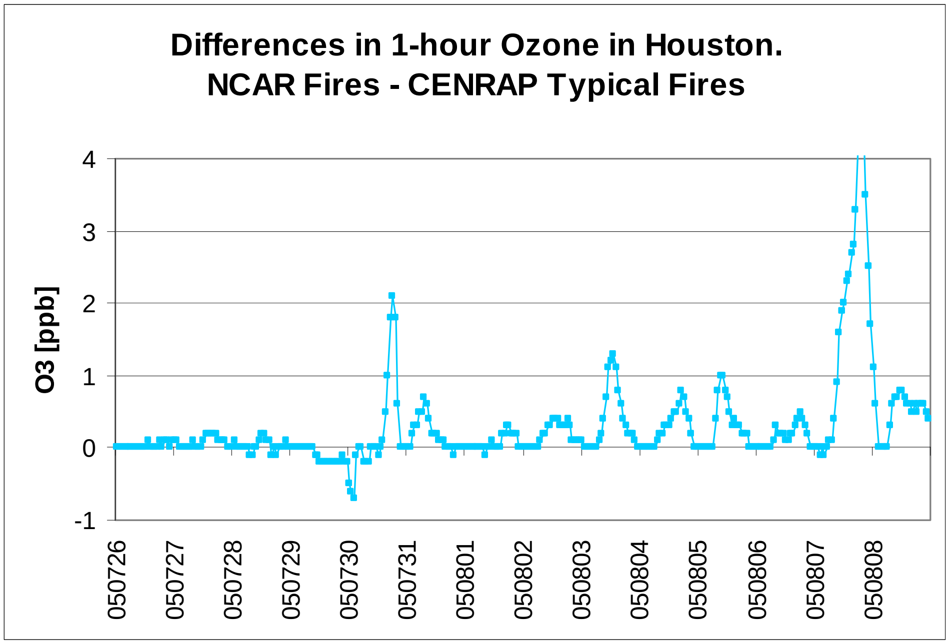


Figure 3-5. Time series of hourly ozone differences in the base year when using NCAR fires instead of CENRAP typical fires.



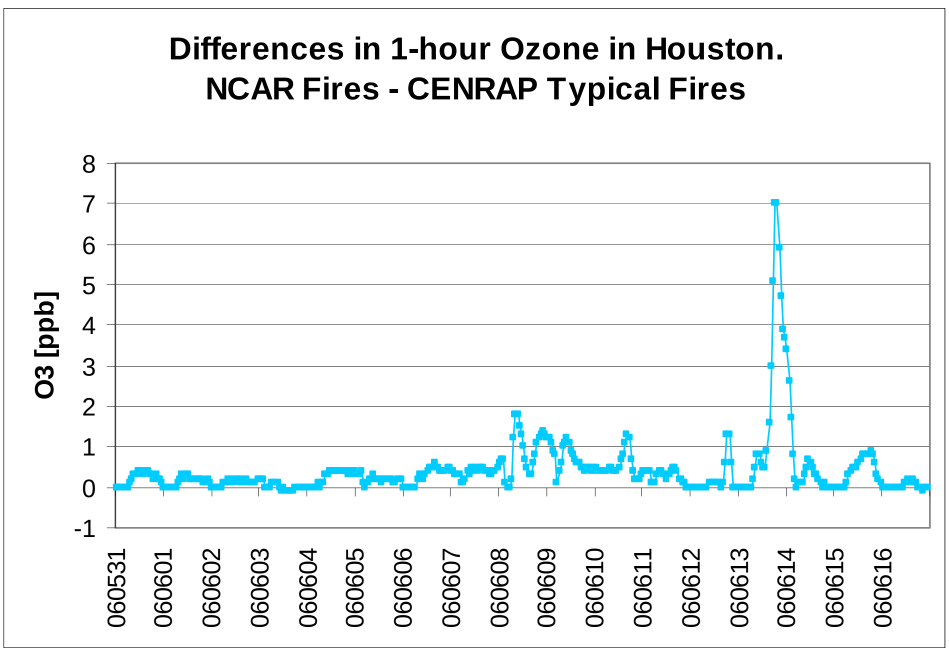
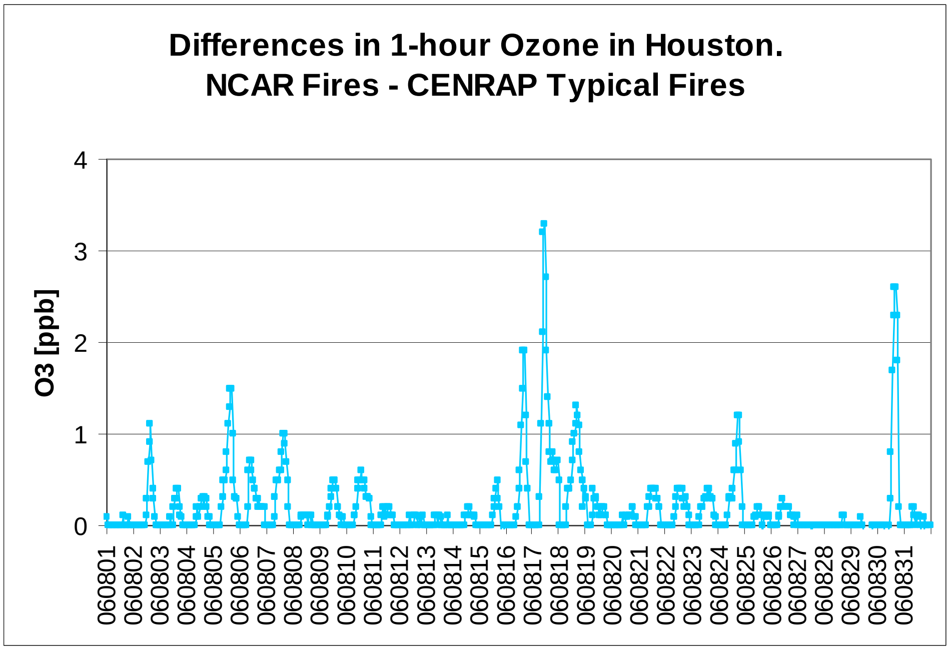


Figure 3-5 (continued). Time series of hourly ozone differences in the base year when using NCAR fires instead of CENRAP typical fires.



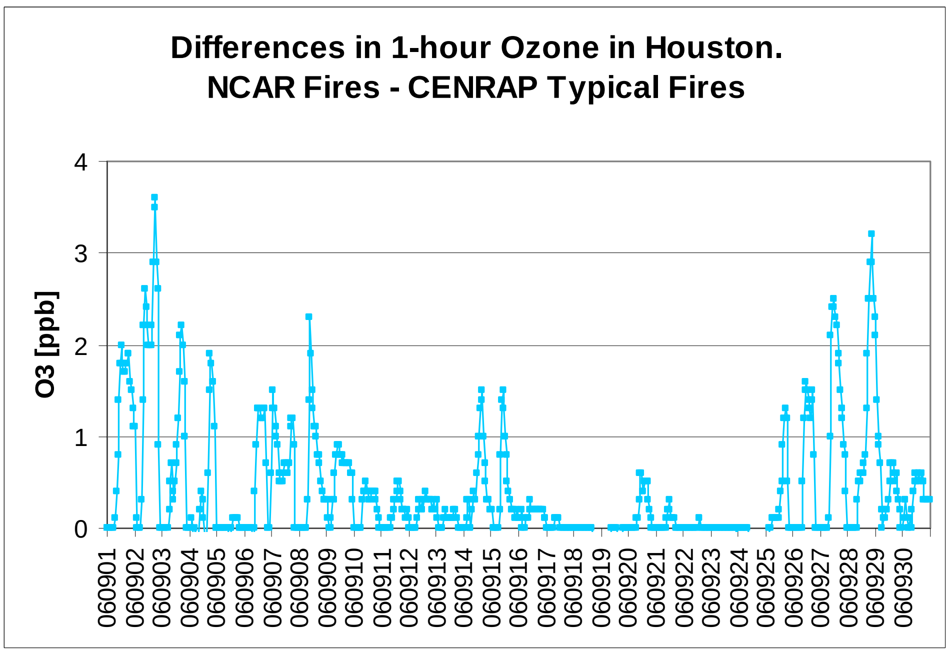


Figure 3-5 (continued). Time series of hourly ozone differences in the base year when using NCAR fires instead of CENRAP typical fires.

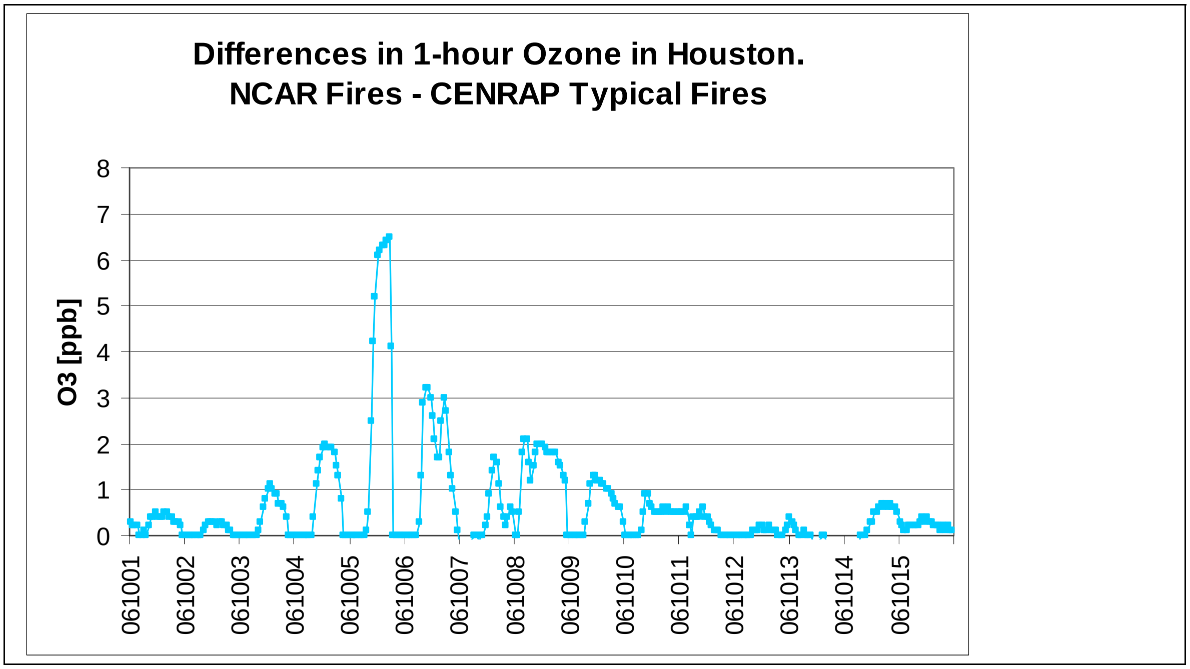


Figure 3-5 (concluded). Time series of hourly ozone differences in the base year when using NCAR fires instead of CENRAP typical fires.

4.0 REFERENCES

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Tai, E.; Jimenez, M.; Nopmongcol, O.; Wilson, G.; Mansell, G.; Koo, B.; Yarwood, G. 2008. "Boundary Conditions and Fire Emissions Modeling." Prepared for Texas Commission on Environmental Quality. September.

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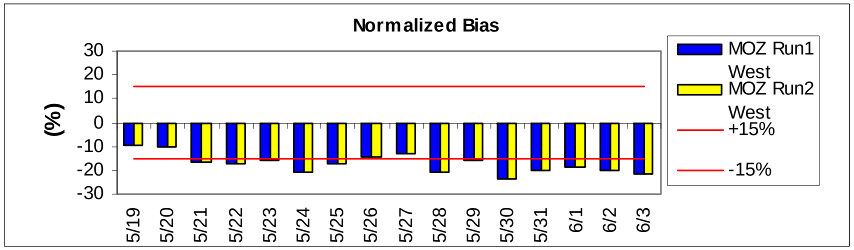
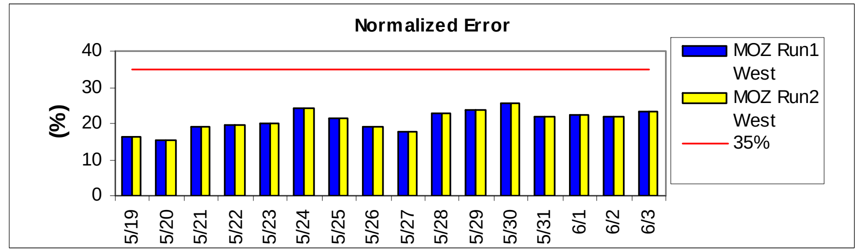
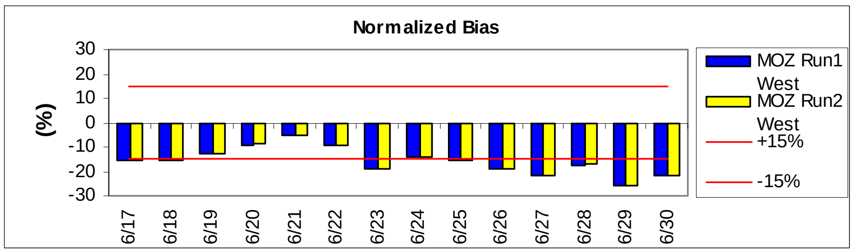
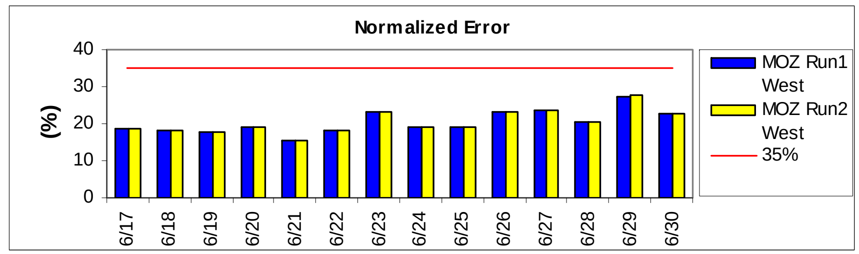
APPENDIX A

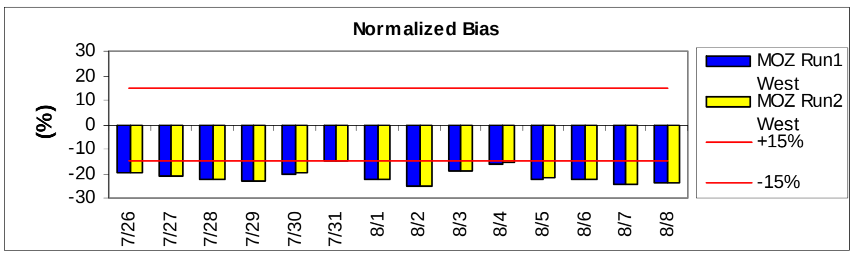
Normalized bias and error of 1-hour ozone at sites near the TCEQ western boundary from the two CAMx runs using MOZART boundary conditions. Run 2 updated the fire emissions from Run 1.

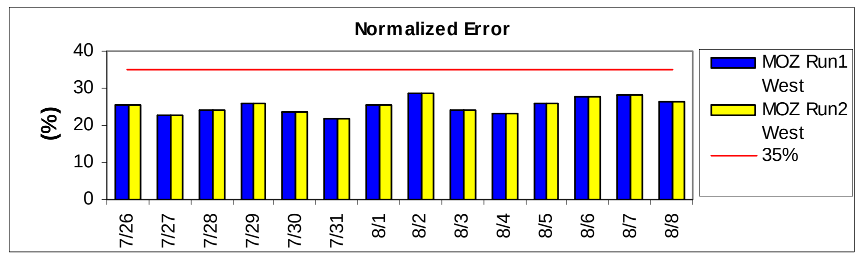


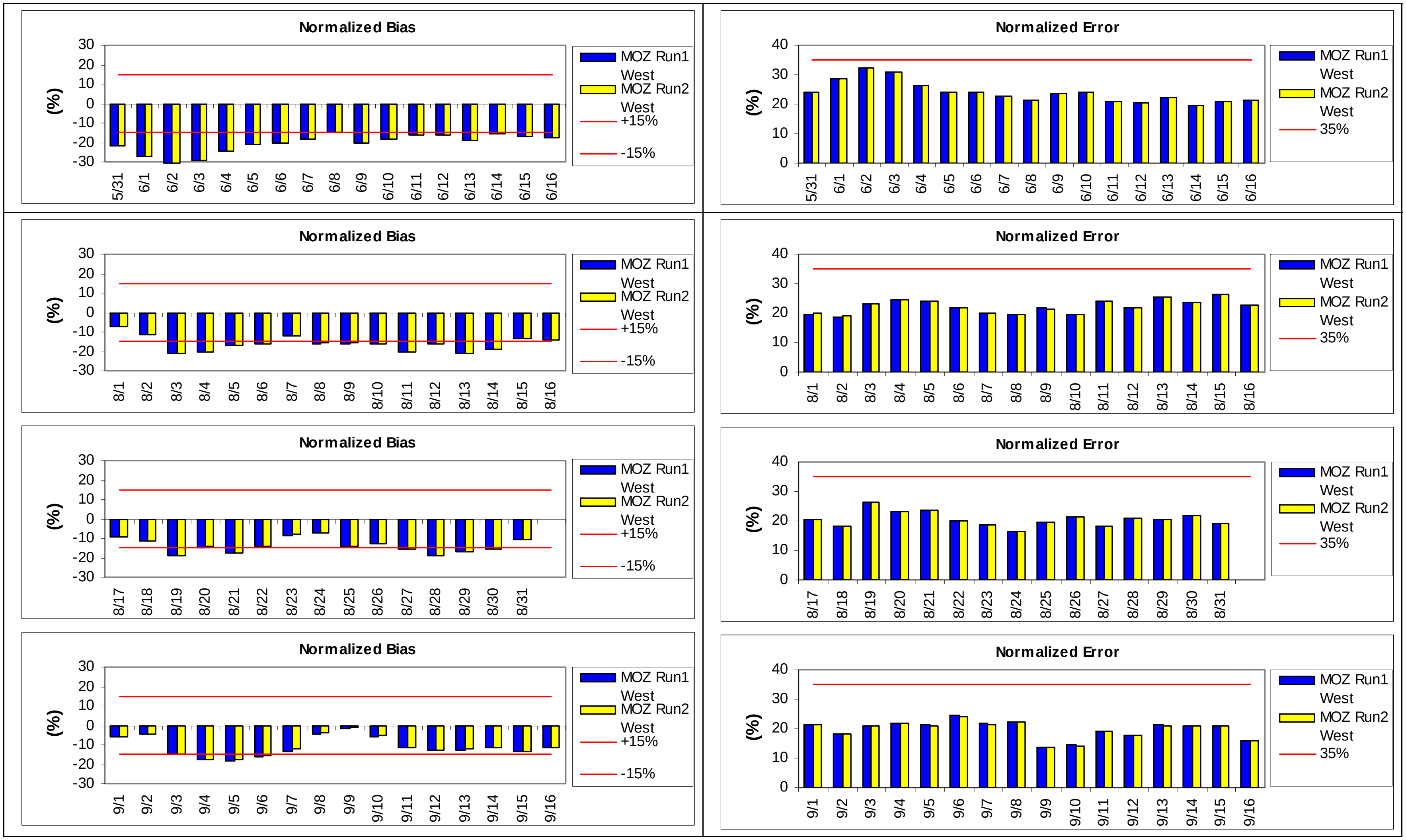











Normalized Bias
(%)
MOZ Run1 West
MOZ Run2 West
+15%
-15%
5/31 6/1 6/2 6/3 6/4 6/5 6/6 6/7 6/8 6/9 6/10 6/11 6/12 6/13 6/14 6/15 6/16
Normalized Error
(%)
MOZ Run1 West
MOZ Run2 West
35%
5/31 6/1 6/2 6/3 6/4 6/5 6/6 6/7 6/8 6/9 6/10 6/11 6/12 6/13 6/14 6/15 6/16
Normalized Bias
8/1 8/2 8/3 8/4 8/5 8/6 8/7 8/8 8/9 8/10 8/11 8/12 8/13 8/14 8/15 8/16
Normalized Error
8/1 8/2 8/3 8/4 8/5 8/6 8/7 8/8 8/9 8/10 8/11 8/12 8/13 8/14 8/15 8/16
Normalized Bias
8/17 8/18 8/19 8/20 8/21 8/22 8/23 8/24 8/25 8/26 8/27 8/28 8/29 8/30 8/31
Normalized Error
8/17 8/18 8/19 8/20 8/21 8/22 8/23 8/24 8/25 8/26 8/27 8/28 8/29 8/30 8/31
Normalized Bias
9/1 9/2 9/3 9/4 9/5 9/6 9/7 9/8 9/9 9/10 9/11 9/12 9/13 9/14 9/15 9/16
Normalized Error
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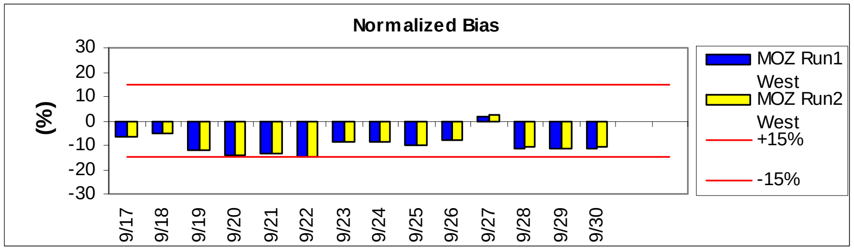
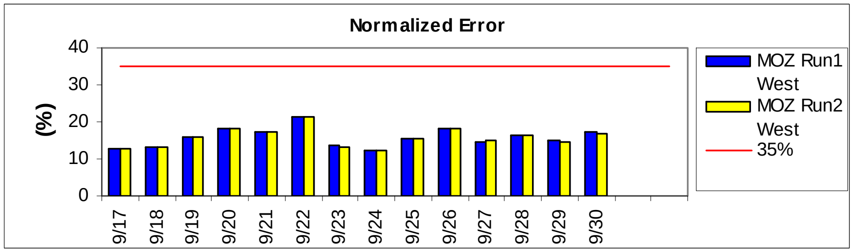
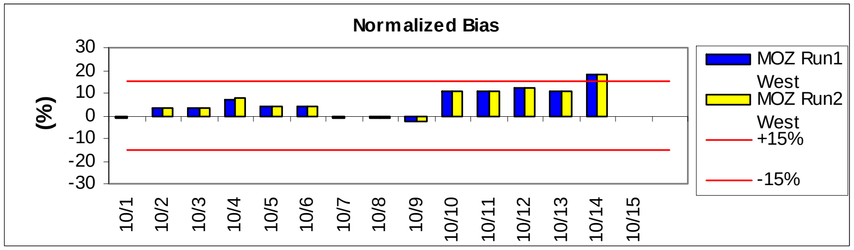
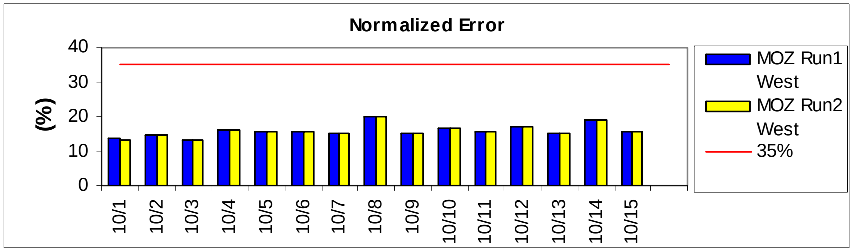

Normalized Bias
(%)
MOZ Run1 West
MOZ Run2 West
+15%
-15%
9/17 9/18 9/19 9/20 9/21 9/22 9/23 9/24 9/25 9/26 9/27 9/28 9/29 9/30

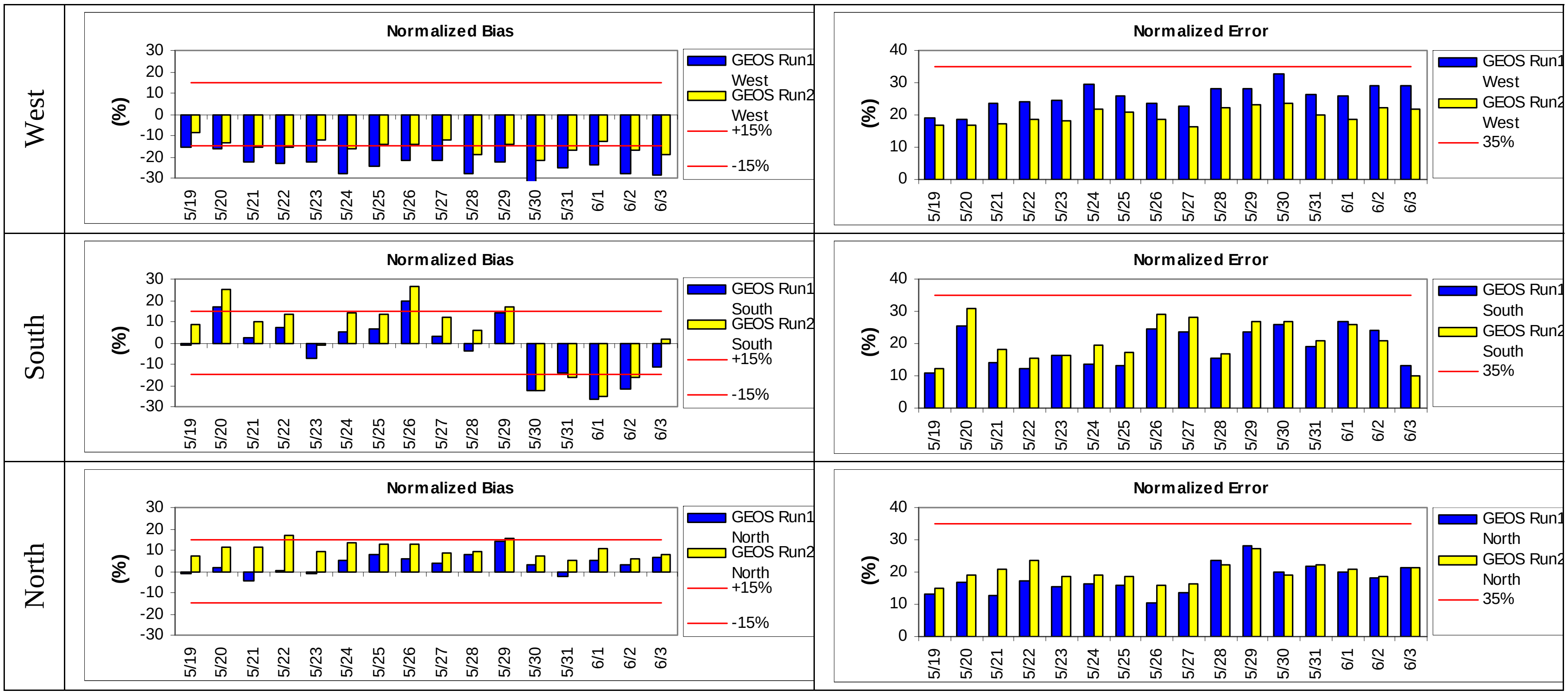

Normalized Error
(%)
MOZ Run1 West
MOZ Run2 West
35%
9/17 9/18 9/19 9/20 9/21 9/22 9/23 9/24 9/25 9/26 9/27 9/28 9/29 9/30


Normalized Bias
(%)
MOZ Run1 West
MOZ Run2 West
+15%
-15%
10/1 10/2 10/3 10/4 10/5 10/6 10/7 10/8 10/9 10/10 10/11 10/12 10/13 10/14 10/15

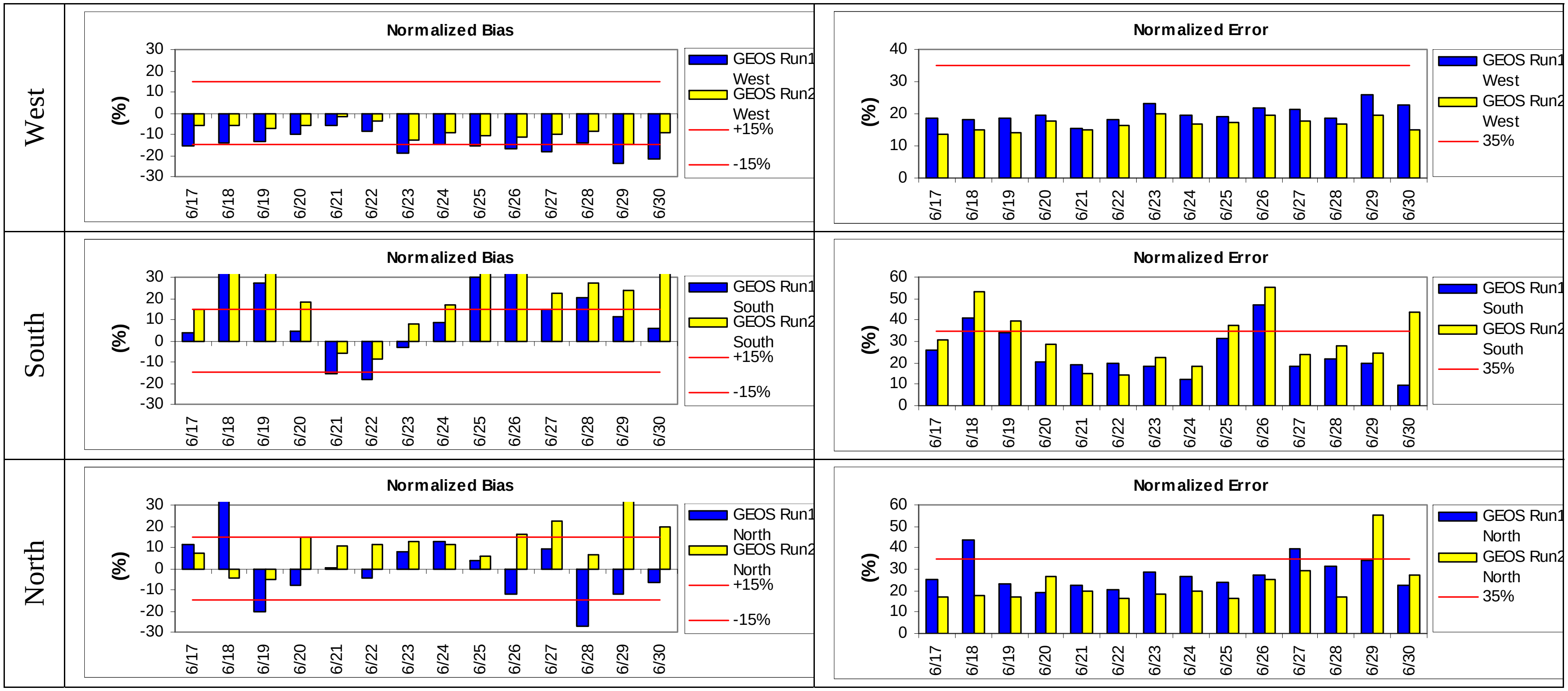

Normalized Error
(%)
MOZ Run1 West
MOZ Run2 West
35%
10/1 10/2 10/3 10/4 10/5 10/6 10/7 10/8 10/9 10/10 10/11 10/12 10/13 10/14 10/15

APPENDIX B

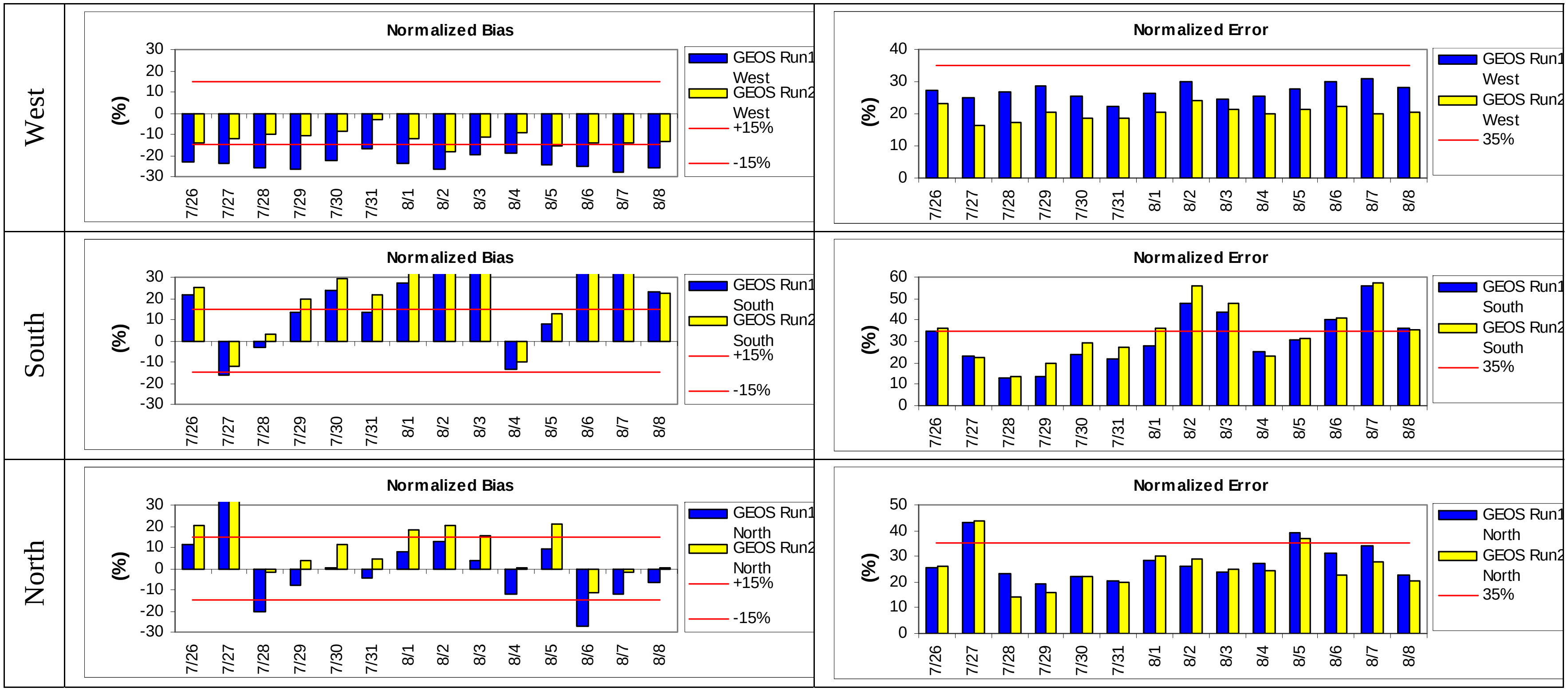
Bar charts of normalized bias and error of 1-hour ozone between two CAMx Runs using GEOS-Chem boundary conditions



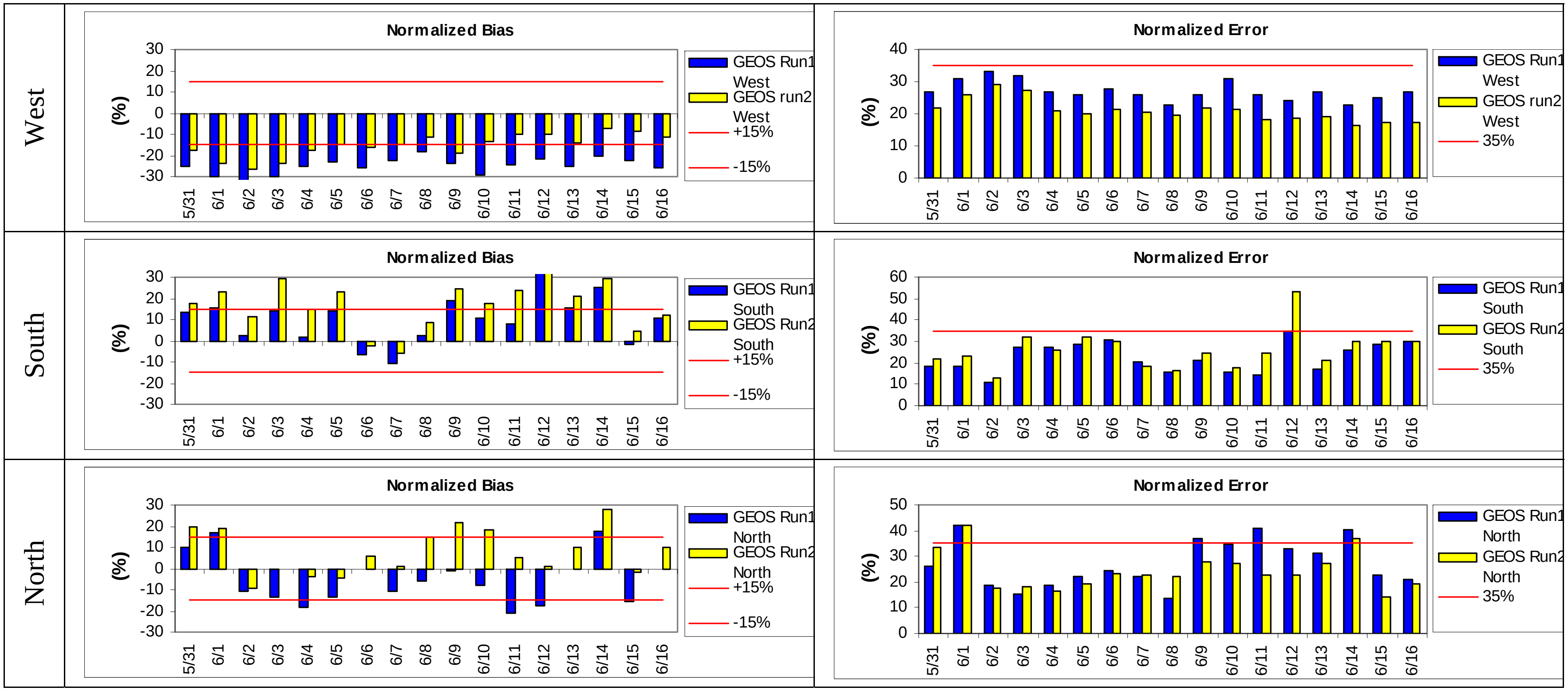
Normalized bias and error for 1-hour ozone at monitors near TCEQ's western, southern, and northern boundaries during the May 19 – June 3, 2005 episode.



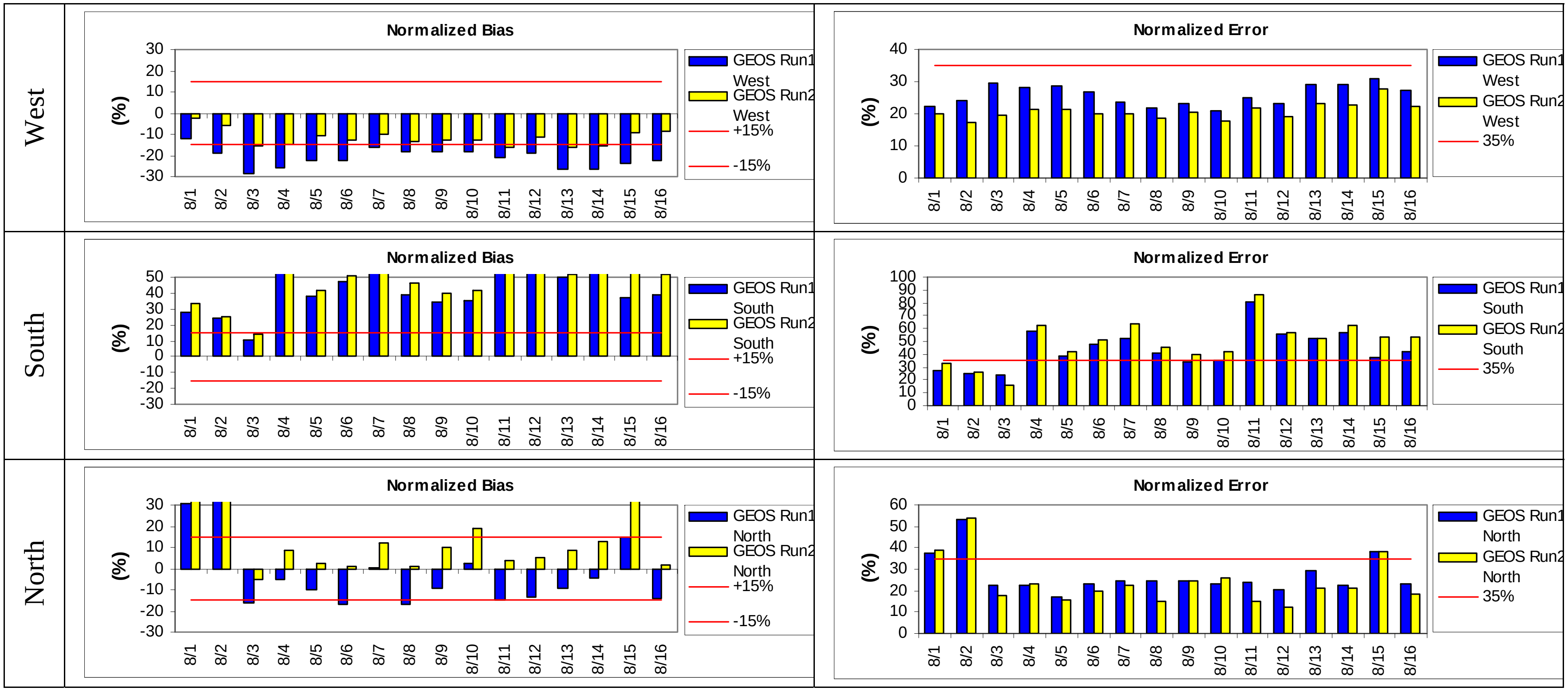
Normalized bias and error for 1-hour ozone at monitors near TCEQ's western, southern, and northern boundaries during the June 17 - 30, 2005 episode.



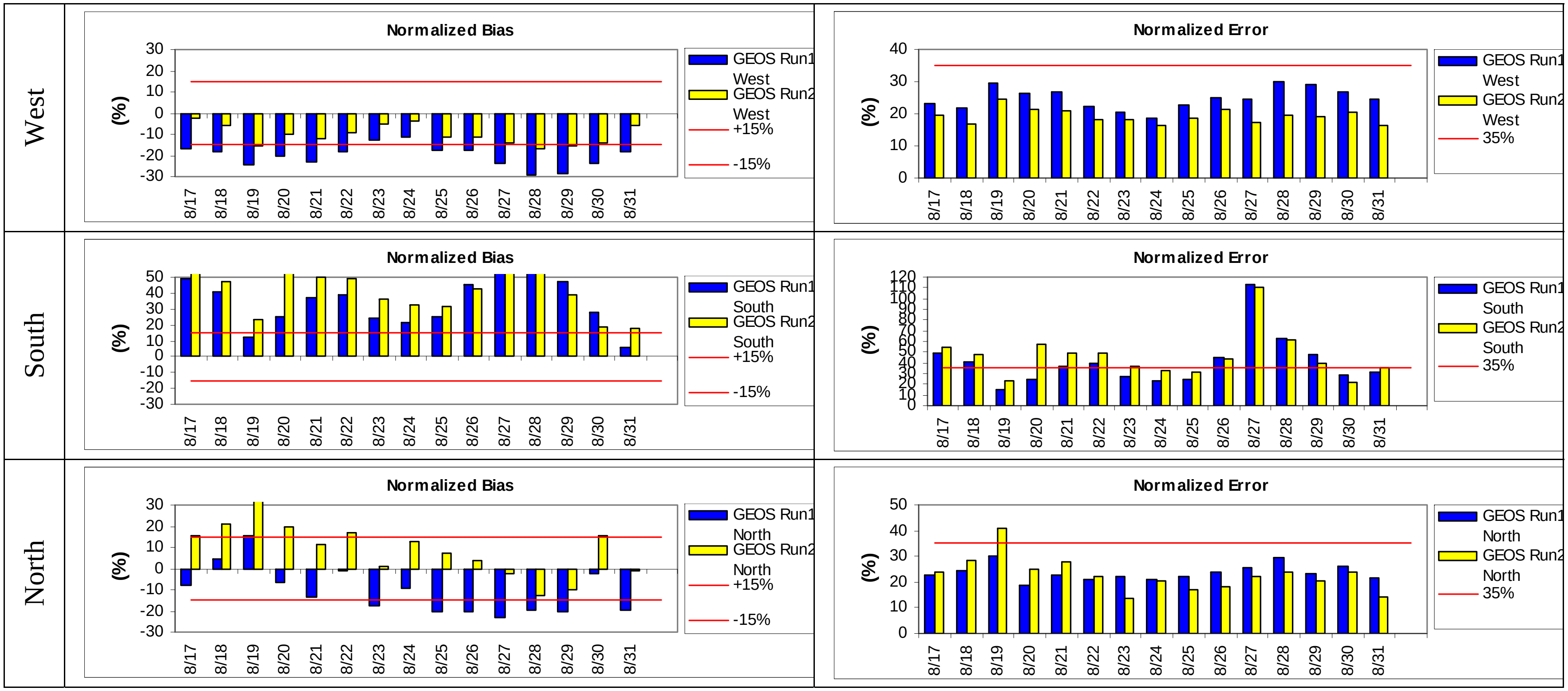
Normalized bias and error for 1-hour ozone at monitors near TCEQ's western, southern, and northern boundaries during the July 26 – August 8, 2005 episode.



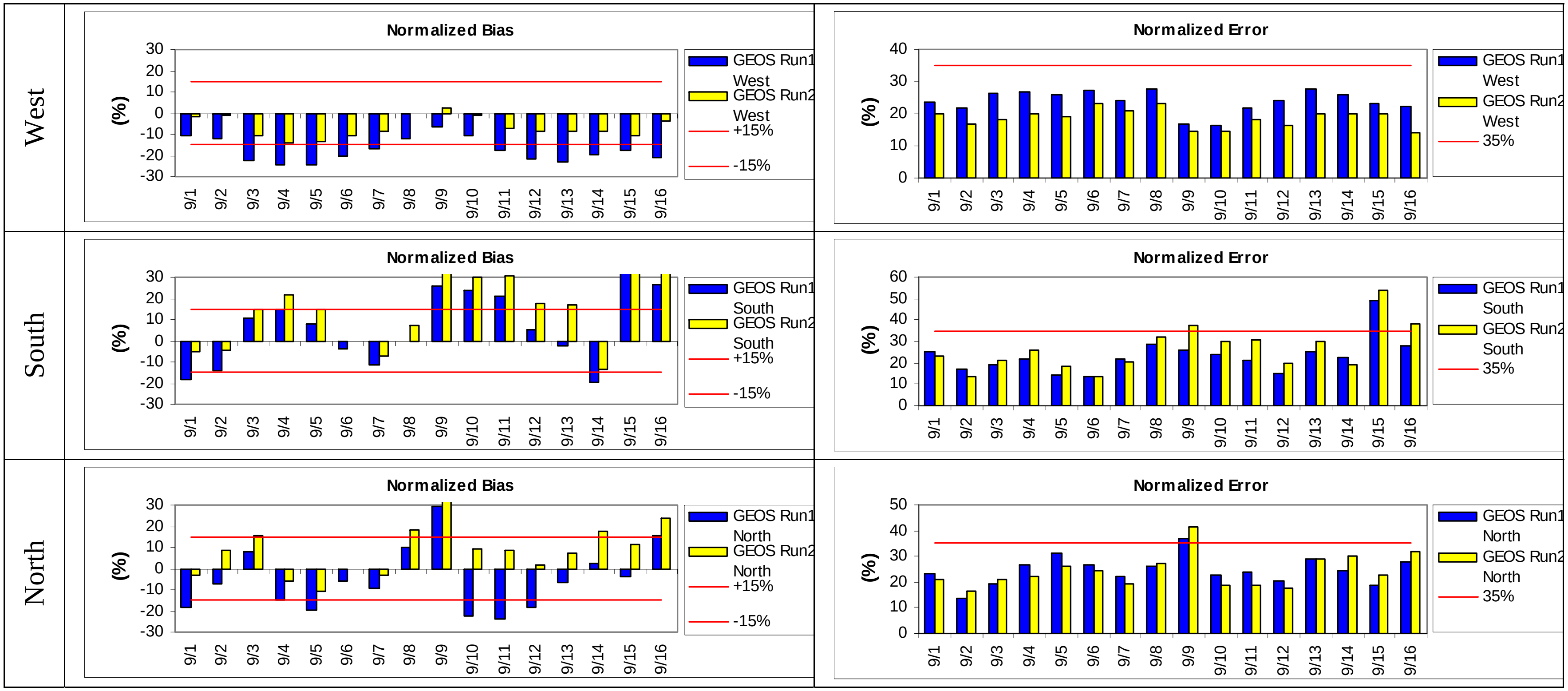
Normalized bias and error for 1-hour ozone at monitors near TCEQ's western, southern, and northern boundaries during the May 31 – June 16, 2006 episode.



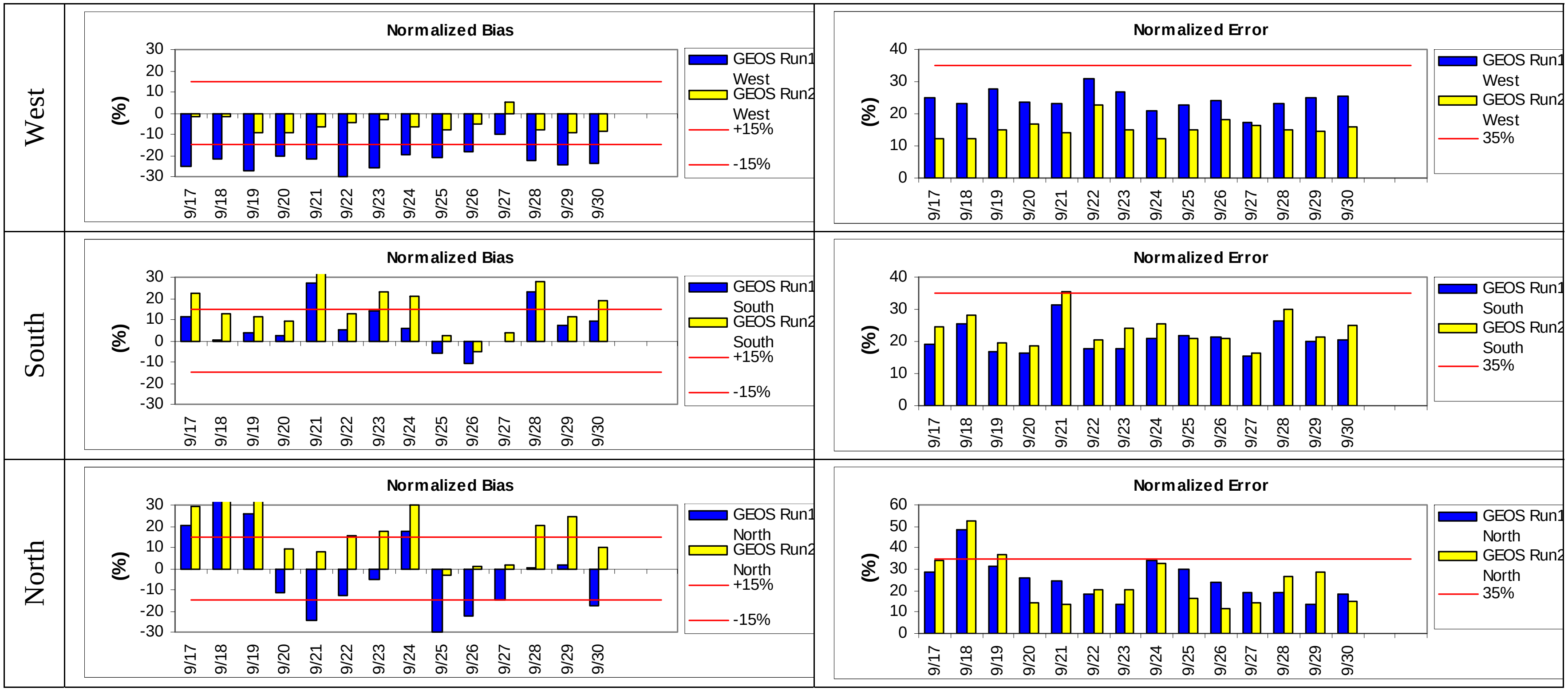
Normalized bias and error for 1-hour ozone at monitors near TCEQ’s western, southern, and northern boundaries during the August 1 – October 15, 2006 episode



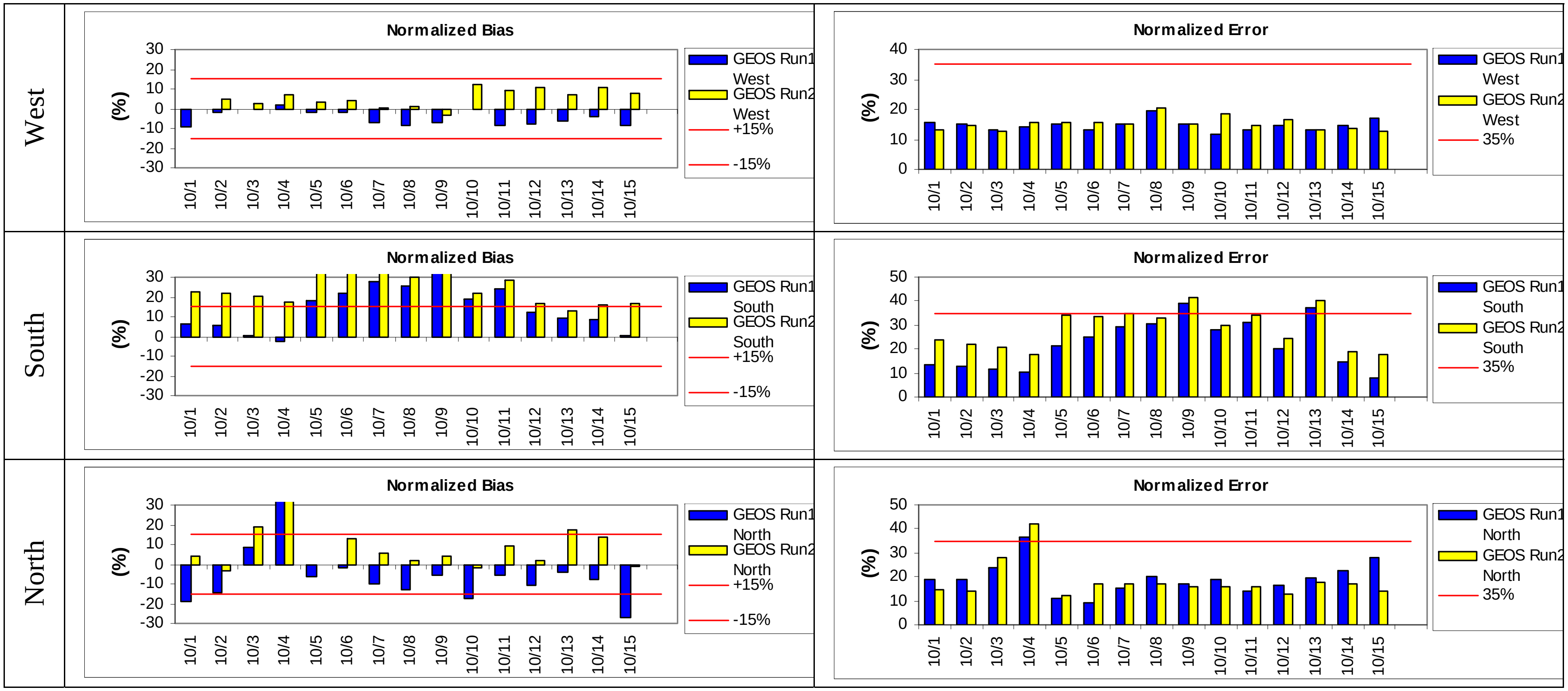
Normalized bias and error for 1-hour ozone at monitors near TCEQ's western, southern, and northern boundaries during the August 1 – October 15, 2006 episode



Normalized bias and error for 1-hour ozone at monitors near TCEQ's western, southern, and northern boundaries during the August 1 – October 15, 2006 episode



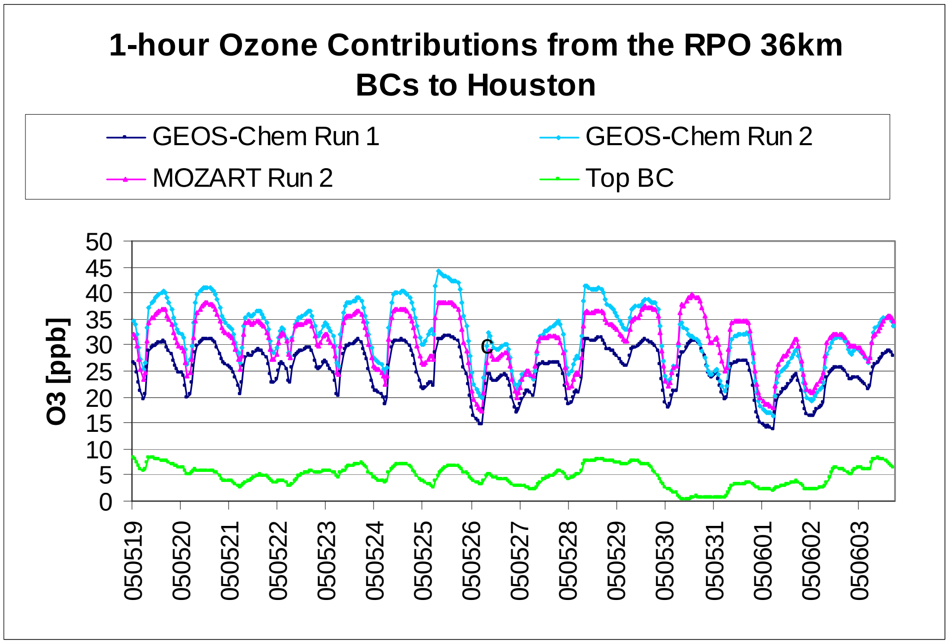
Normalized bias and error for 1-hour ozone at monitors near TCEQ's western, southern, and northern boundaries during the August 1 – October 15, 2006 episode

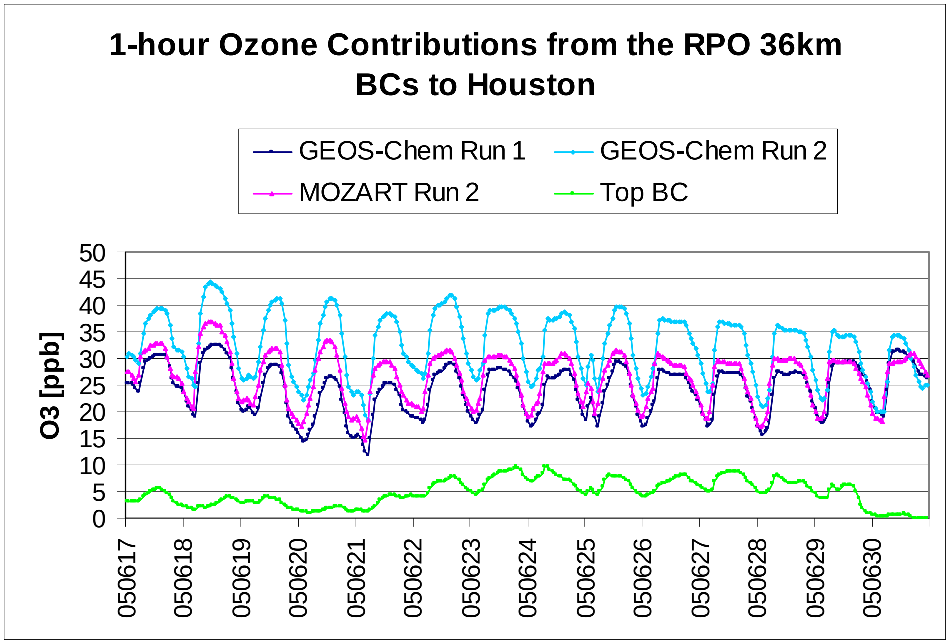


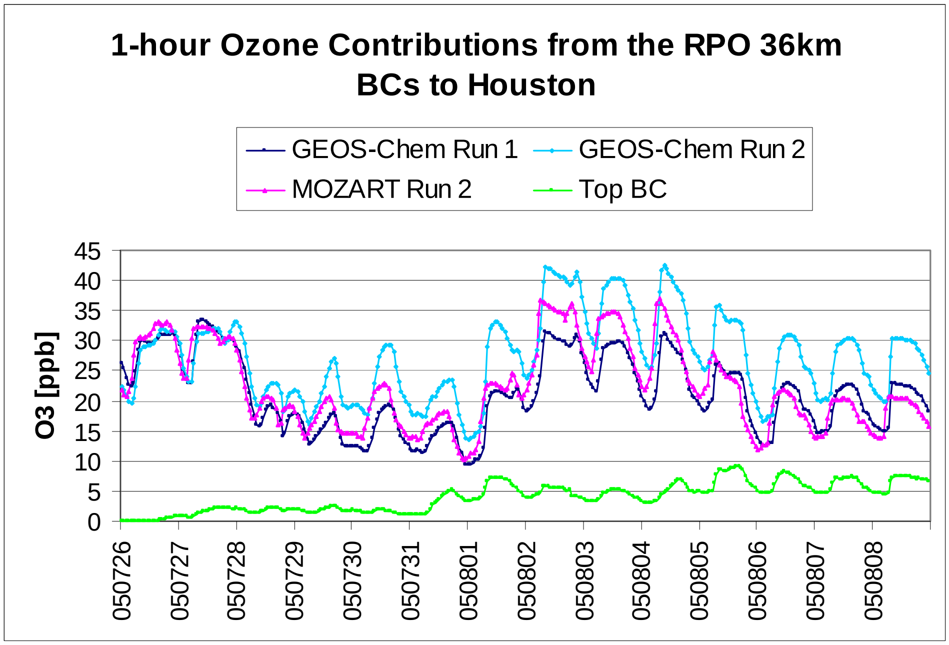
Normalized bias and error for 1-hour ozone at monitors near TCEQ's western, southern, and northern boundaries during the August 1 – October 15, 2006 episode

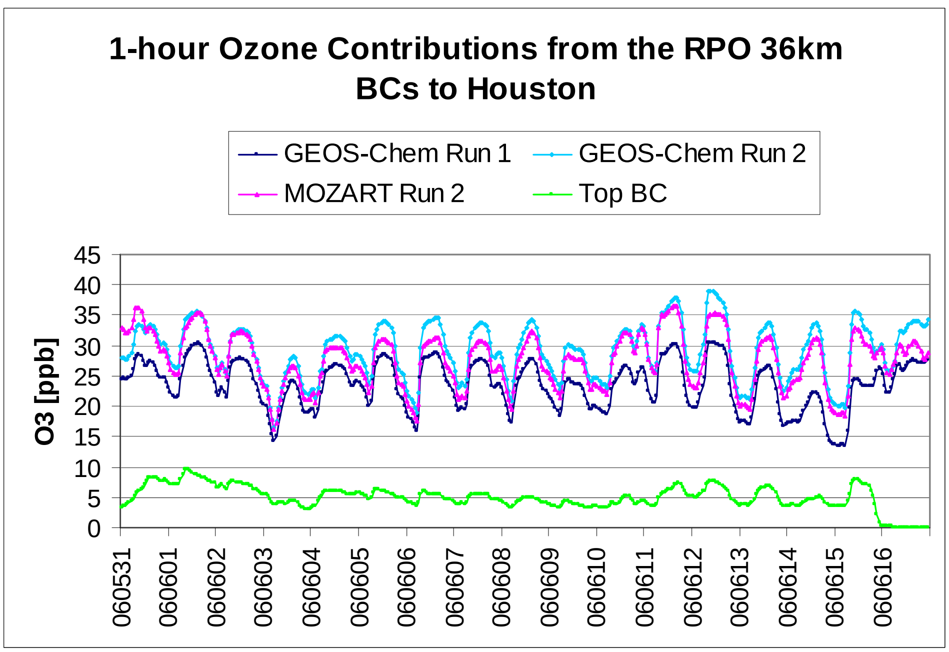
APPENDIX C

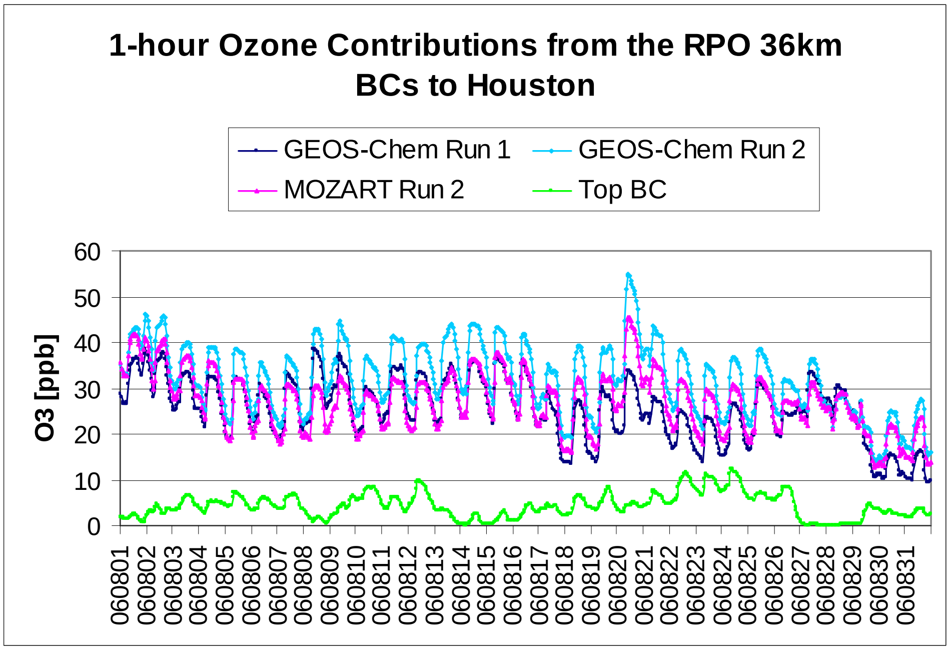
Time series of inert ozone contributions from the RPO 36 km lateral boundaries to Houston



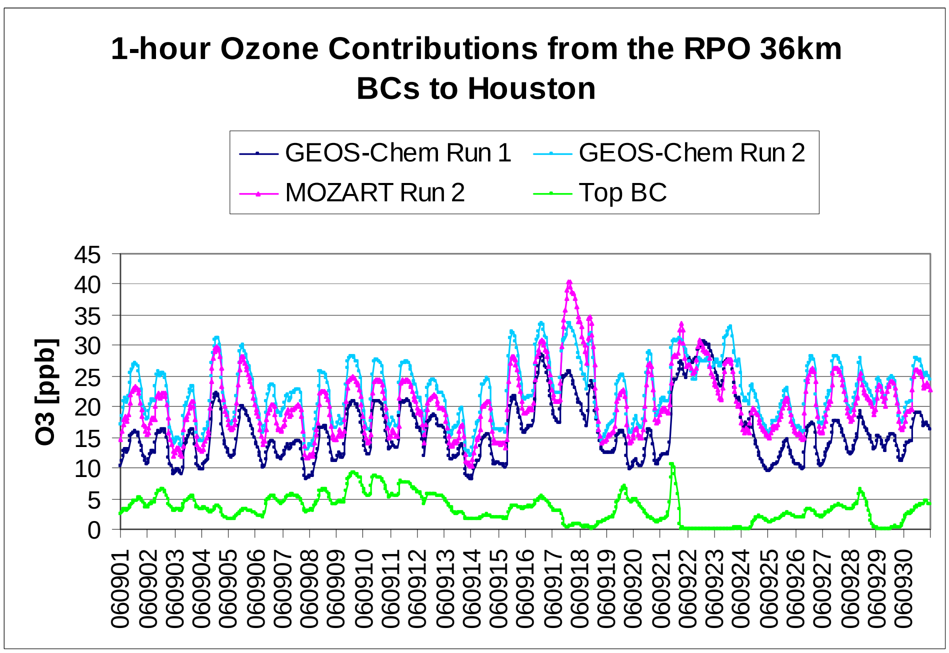



1-hour Ozone Contributions from the RPO 36km BCs to Houston
GEOS-Chem Run 1
GEOS-Chem Run 2
MOZART Run 2
Top BC
O3 [ppb]
45
40
35
30
25
20
15
10
5
0
050726
050727
050728
050729
050730
050731
050801
050802
050803
050804
050805
050806
050807
050808

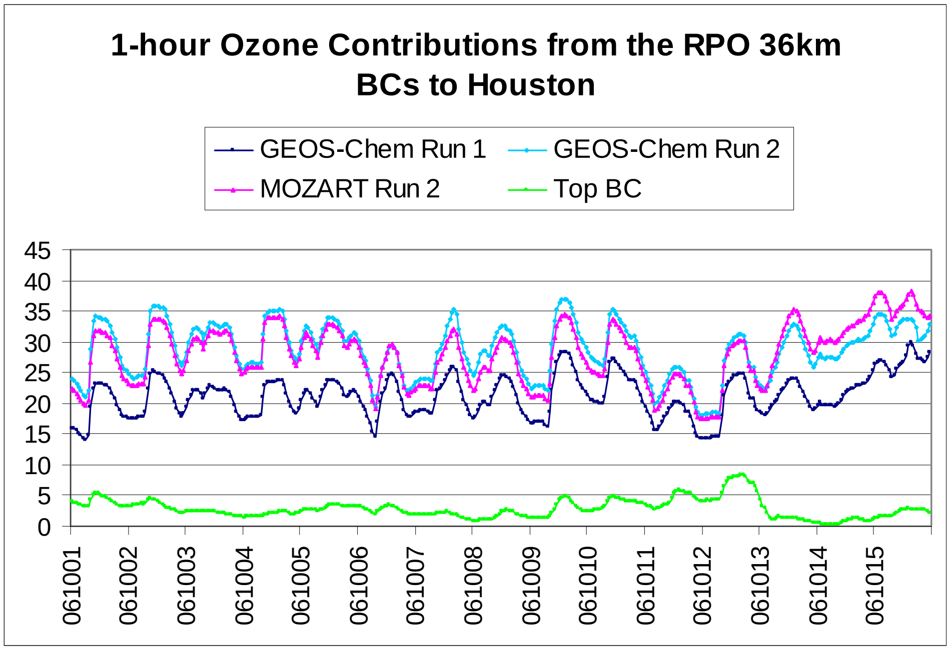

1-hour Ozone Contributions from the RPO 36km BCs to Houston
GEOS-Chem Run 1
GEOS-Chem Run 2
MOZART Run 2
Top BC
O3 [ppb]
45
40
35
30
25
20
15
10
5
0
060531
060601
060602
060603
060604
060605
060606
060607
060608
060609
060610
060611
060612
060613
060614
060615
060616



1-hour Ozone Contributions from the RPO 36km BCs to Houston
GEOS-Chem Run 1
GEOS-Chem Run 2
MOZART Run 2
Top BC
O3 [ppb]
60
50
40
30
20
10
0
060801
060802
060803
060804
060805
060806
060807
060808
060809
060810
060811
060812
060813
060814
060815
060816
060817
060818
060819
060820
060821
060822
060823
060824
060825
060826
060827
060828
060829
060830
060831



1-hour Ozone Contributions from the RPO 36km BCs to Houston
GEOS-Chem Run 1
GEOS-Chem Run 2
MOZART Run 2
Top BC
O3 [ppb]
45
40
35
30
25
20
15
10
5
0
060901
060902
060903
060904
060905
060906
060907
060908
060909
060910
060911
060912
060913
060914
060915
060916
060917
060918
060919
060920
060921
060922
060923
060924
060925
060926
060927
060928
060929
060930


1-hour Ozone Contributions from the RPO 36km BCs to Houston
GEOS-Chem Run 1
GEOS-Chem Run 2
MOZART Run 2
Top BC
45
40
35
30
25
20
15
10
5
0
061001
061002
061003
061004
061005
061006
061007
061008
061009
061010
061011
061012
061013
061014
061015