Final Report

SENSITIVITY ANALYSES OF THE SEPTEMBER 8-11, 1993 OZONE EPISODE USING HIGH RESOLUTION RAMS METEOROLOGY

Work Order No. 31984-22
TNRCC Umbrella Contract No. 582-0-31984

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1. INTRODUCTION

TNRCC is responsible for developing a State Implementation Plan (SIP) for ozone in Houston/Galveston and Beaumont/Port-Arthur (HGBPA) ozone nonattainment areas (the Houston area). The TNRCC's SIP relies upon photochemical modeling to relate atmospheric ozone concentrations to emission levels for ozone precursors. The most recent modeling was performed using the Comprehensive Air Quality Model with extensions (CAMx) version 2.03 for the December, 2000 SIP revision and considered emissions of volatile organic compounds (VOCs), nitrogen oxides (NOx) and carbon monoxide. Since then a number of new features have been implemented in the CAMx modeling system, in particular, flexi-nesting and chlorine chemistry. Recent studies (ENVIRON, 2001; Tanaka, 2000) have suggested that reactive chlorine compounds may play a significant role in ozone formation in the Houston atmosphere, while the use of the flexi-nesting features of the CAMx model may be able to provide significant model performance improvements for the Houston area. In addition, during the summer of 2000 the Texas Air Quality Study (TexAQS) was conducted to collect atmospheric measurements of ozone and ozone precursors in order to further support atmospheric computer modeling of the Houston area as well as to better characterize industrial precursor emissions within the area. The impacts on simulated ozone concentrations due to these new features of the CAMx model as well as the analysis of future year alternative emission scenarios have been investigated and documented previously using the SAIMM meteorological fields (ENVIRON, 2002; 2002a; 2002b). The purpose of the current study is to apply the CAMx model to the 8-11 September, 1993 ozone episode using alternative meteorological fields from the RAMS model and to evaluate model performance under alternative emission scenarios. In addition, the modeling effort will focus on the determination of alternative VOC emission reductions that would be required to compensate for relaxing the NOx reductions currently implemented in the future year Strategy I8a.

OBJECTIVES

The overall objectives of this study are as follows:

1. Apply the CAMx model to the 8-11 September, 1993 ozone episode and evaluate model performance using the latest meteorological fields developed using the Regional Atmospheric Modeling System (RAMS). A model performance evaluation using the statistical and graphical analyses recommended by EPA Guidance will be conducted and the modeling results and model performance are compared with that obtained using the SAIMM meteorological data.

2. Perform sensitivity analyses in order to assess model performance under alternative emissions scenarios. The various alternative emission scenarios are developed to reflect a realistic estimate of VOC emission levels consistent with the TexAQS analysis. The alternative emission scenarios were developed based on TNRCC recommendations.

3. Determine whether less stringent industrial NOx emission reductions in the 2007 Strategy I8a scenario could be compensated by greater reductions in 2007 industrial VOC emissions.

2. MODELING DATABASES AND MODEL CONFIGURATION

This section of the report documents the Houston ozone modeling databases that were utilized, the CAMx model configuration and options used to perform the emission sensitivity simulations, and the implementation of the CAMx model.

CAMx MODELING DATABASES

The TNRCC has developed CAMx modeling databases for ozone episodes that occurred in 1993 during the COAST field study. The episode periods are September 6-11 and August 16-20, 1993. Several concerns have been raised about the performance of modeling using these databases, and the TNRCC did not use the August episode in the HGBPA SIPs (the TNRCC is currently developing new modeling episodes). The TNRCC has also performed Houston modeling over a much larger area referred to as the SuperCOAST domain. The modeling performed for the current study utilizes the SuperCOAST domain with an inner 2-way nested 4-km grid which is the same as the 4-km grid used in the original COAST domain. In addition, a high-resolution 1.33-km flexi-nested grid is included to better simulate the relatively high density of point source emissions within the industrial areas along the Houston Ship Channel and Galveston Bay. The area covered by the CAMx model for the SuperCOAST domain is shown in Figure 2-1. The domain has an outer 16-km grid with an inner 2-way nested 4-km grid. The grid is defined in UTM zone 15 coordinates and has 11 vertical layers between the surface and 3.03 km. with a surface layer ~20 meters deep. Figure 2-2 displays the location of the 1.33-km grid within the 4-km HGBPA grid. Note that previous studies have used the 1.33-km grid with CAMx flexi-nesting to interpolate meteorology from the 4-km to 1.33-km, but in this study 1.33-km meteorology was explicitly generated by the RAMS model.

The COAST domain meteorological fields for both the August and September 1993 episodes were developed using the SAIMM hydrostatic meteorological model with data assimilation (Kessler and Douglas, 1992). SAIMM was applied with relatively strong assimilation of wind data in an attempt "nudge" the model into reproducing the timing and magnitude of the land/sea breezes (Lolk et al., 1995). This has raised some concerns that the strength of the nudging may have compromised the consistency of the meteorological fields (Yocke et al., 1996). Numerous recent studies have developed alternate meteorological fields for the September Episode using other mesoscale meteorological models and horizontal resolutions (Emery et al., 2001; Tremback and Emery, 2001) and CAMx model performance evaluations using these alternative meteorological fields have been performed and documented (Tesche and McNally, 2001). The CAMx 1993 base case model simulations and future year emission sensitivity simulations using the SAIMM meteorological fields have been documented previously (ENVIRON, 2002).

In August 2001, ENVIRON and Mission Research Corporation/ASTER completed high-resolution meteorological simulations of the September 1993 COAST ozone episode for the TNRCC (Tremback and Emery, 2001). The model simulations utilized the Regional Atmospheric Modeling System (RAMS) and included a 1.33-km high-resolution nested grid domain over the Houston Ship Channel and Galveston Bay. Numerous simulations were performed to assess the sensitivity to model configuration and performance optimization. The current study extends previous similar analyses and investigates the CAMx model performance and future year emission sensitivity analyses using the RAMS meteorological fields developed by Tremback and Emery (2001). A detailed description and analysis of the RAMS simulations, including model configuration, options and model performance evaluation can be found in

Tremback and Emery (2001). The RAMS run denoted "r4" by Tremback and Emery (2001) was used to develop CAMx input files for this study. CAMx was run in a UTM Zone 15 coordinate system to match the available emission inventories, and so RAMS meteorological fields were translated from their native Polar Stereographic grid to the CAMx UTM grid using ENVIRON's RAMSCAMx software.

The base case emission inventories were developed by the TNRCC and have undergone continual upgrades to include the latest information with the September episode inventories being the most updated as it continues to be used for SIP modeling. A discussion of the various components of the inventories, including data sources and development methodologies is presented in the final report for a previous TNRCC sponsored project: Sensitivity Analyses of the September 8-11, 1993 Ozone Episode, Work Order NO. 31984-19, TNRCC Umbrella Contract NO. 582-0-31984 (ENVIRON, 2002). Boundary and initial conditions were developed by the TNRCC using methods developed in Yocke et al., 1996.

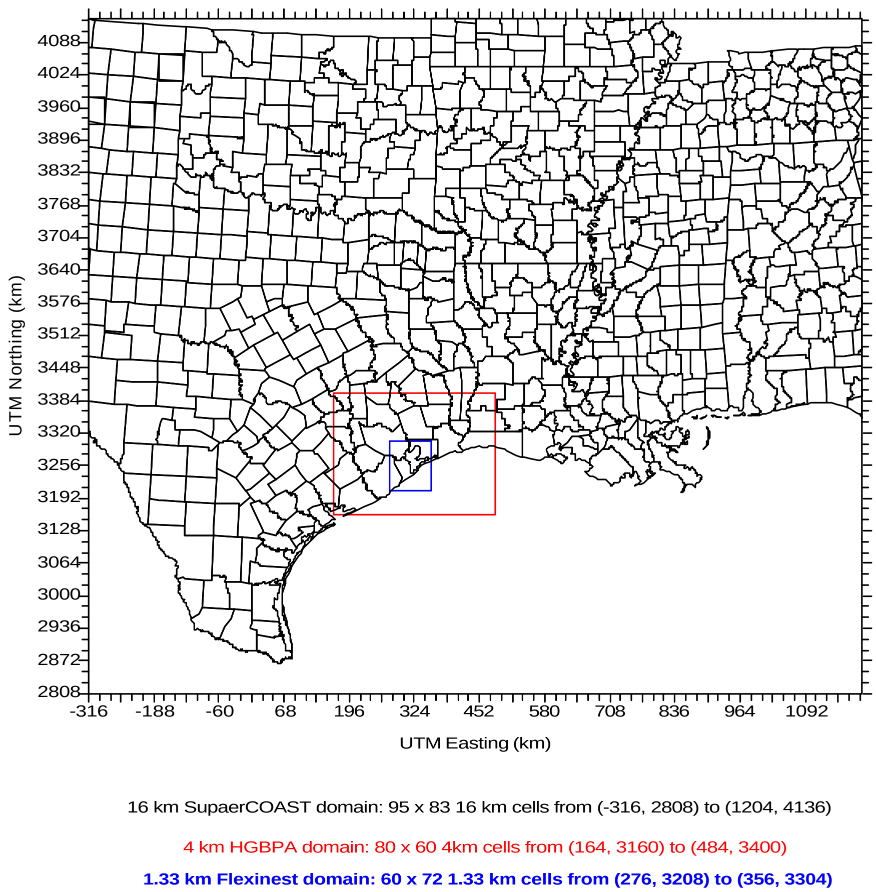

Figure 2-1. Map of the SuperCOAST domain showing the location of the 4-km HGBPA and 1.33 km domains.

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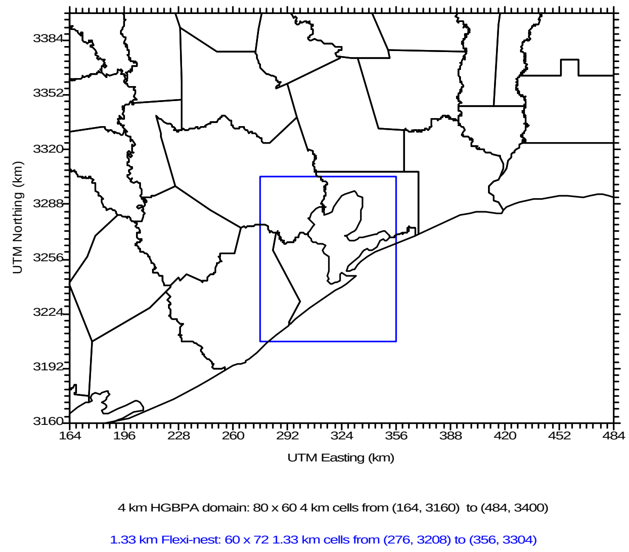

Figure 2-2. Map of the 4-km HGBPA domain showing the location of the 1.33-km grid.

CAMx MODEL CONFIGURATION

The TNRCC SIP modeling simulations for the 1993 ozone episodes were performed using the Comprehensive Air Quality Model with extensions (CAMx) version 1.13. Under Work Order No. 31984-19 (ENVIRON, 2002; 2002a) ENVIRON investigated the sensitivity of the simulation results to model version and configurations for both the 1993 base case and future year 2007 base case. The results of these sensitivity simulations are documented in ENVIRON, 2002a. This study led to the recommendation to use version 3.01 of the CAMx model for further emission sensitivity simulations. The model configuration makes use of the updated chlorine chemistry and includes the 1.33-km Houston nested grid domain. In order to adequately simulate the interaction of NOx and VOC emission within the industrial area within and around the Houston Ship Channel and Galveston Bay, the Plume-in-Grid treatment of large NOx sources should not be implemented. Finally, the advection scheme used in the simulations should be the Piecewise Parabolic Method (PPM) in order to minimize the overly diffusive effects seen with the Smolarkiewicz solver. Thus, the starting point for the emission sensitivity simulations documented herein is the CAMx version 3.01 with chlorine chemistry including the 1.33-km nested grid domain, the PPM advection scheme and no Plume-in-Grid treatment of elevated point source emissions.

EMISSION INVENTORIES

As was the case with the previous study (ENVIRON, 2002a; 2002b), the objective of the current study was to perform various emission sensitivity analyses and to assess model performance under alternative emission scenarios for the September 1993 base year ozone episode using the latest RAMS meteorology including the high resolution 1.33-km nested grid. For the future year Strategy I8a scenario, an investigation of greater industrial VOC emission reductions required to compensate for less stringent industrial NOx emission reductions contained in the final 2000 SIP was also conducted. The alternative emission scenarios examined the effect of increased emissions of volatile organic compounds from industrial sources (industrial VOC, or IVOC).

The specific emission adjustment were made in consultation with TNRCC staff and were intended to approximate realistic levels of VOC emissions consistent with the results of the Texas Air Quality Study of 2000 (TexAQS 2000).

The alternative emission scenarios focused on the HGBPA 4-km nested grid of the modeling domain as this region encompasses the urban areas within and around Houston, as well as the Ship Channel and Galveston Bay. As noted in earlier studies, due to the use of model-ready emission inventory data files, it was not possible to specifically identify individual sources as either industrial or non-industrial. Therefore, for the purposes of the present study, industrial sources are defined simply as all point sources, both elevated and low level. The development of the alternative emission scenarios were accomplished using the EPS2 utility processors to apply appropriate adjustment factors to the elevated and low level NOx and/or VOC emissions.

All alternative emission scenarios considered involved adjustments to industrial olefins within the 8-county Houston-Galveston area only and excluded shipping emissions. In the case of future year scenarios, the emission adjustments considered both existing and new sources for the purpose of adjusting NOx emission levels from the 90% reductions in the SIP. The specific procedures used for developing the emission sensitivity scenarios are documented in ENVIRON, 2002a.

This section of the report summarizes the alternative emission scenarios for both the 1993 base year and future year 2007 Strategy I8a to be applied for the September 1993 SuperCOAST CAMx ozone air quality modeling.

1993 Base Year Emission Scenarios

As noted above, the objective of the current task was to evaluate model performance under various alternative emission scenarios involving continuous industrial VOC (IVOC) emission increases. To provide some reference with respect to the NOx and VOC emissions levels within and outside the HGBPA 4-km grid, Table 2-1 presents a summary of existing emissions in the September 1993 base year emission inventory.

Table 2-1. NOx and VOC 1993 Base Year Emission Summaries within and outside the HGBPA 4-km Domain.

HGBPA 4-km Domain. Emission Component	Inside 4-km Domain (tpd)	Outside 4-km Domain (tpd)
Elevated Point NOx	989	6283
Low Level Point NOx	45	--
Area/Mobile/Biogenic NOx	845	9478 (incl. low level points)
Elevated Point VOC	172	1174
Low Level Point VOC	427	--
Area/Mobile/Biogenic VOC	4039	68559 (incl. low level points)

The emission adjustments considered increases industrial light olefins (IOLE, represented by modeled species ETH and OLE). In consultation with TNRCC staff, the sensitivity scenario for continuous IOLE emission increases identified for evaluation was selected to be the 6xIOLE scenario, consistent with the alternative emission scenarios performed with the MM5 meteorology (ENVIRON, 2002b). The emission scenario was developed through application of the appropriate adjustment factors using the emission processing utilities, MRGUAM and PTSCOR for low level and elevated point sources, respectively, as described in ENVIRON, 2002b. This scenario was simulated using the CAMx air quality model and the resulting model performance was evaluated with respect to EPA guidance on acceptable model performance.

2007 Future Year Emission Scenarios

The objective of the 2007 Strategy I8a emission sensitivity scenarios was to investigate the potential for offsetting the adopted reduction in point source NOx with reductions in industrial VOC emissions. In addition, the effects of the alternative VOC emission scenarios performed for the 1993 Base year simulations were considered for the 2007 Strategy I8a emission scenarios.

In order to accomplish this task, the industrial NOx emission for the I8a scenario were first increased by a factor of 2 to approximate the NOx emission levels with 80% rather than 90% reduction applied to industrial sources. A series of emission scenarios were then developed with varying reductions in industrial olefin (IOLE) emission levels. The CAMx model was applied to determine the extent to which the modeled ozone concentrations could be reduced to the Strategy I8a levels through reduction of industrial olefin emissions. As noted above, the procedures used to develop the emission scenarios were subsequently refined to apply only within the 8-county region with appropriate treatment of sources not subject to controls.

For reference, Table 2-2 presents to VOC and NOx emission totals within and outside the HGBPA 4-km modeling domain. Table 2-3 provides a summary of the industrial NOx and VOC/OLE emission reduction scenarios considered. Note that the “80nox.*ole” scenarios represent the 2007 future year emission levels without the SIP adopted NOx reductions and represent the starting point for the investigation of potential IOLE reduction scenarios to compensate for the proposed NOx reductions. Of note is the “80nox00ole” scenario, which corresponds to the maximum potential industrial olefin emission reductions.

Table 2-2. NOx and VOC Strategy I8a Emission Summaries within and outside the HGBPA 4-km Domain.

HGBPA 4-km Domain. Emission Component	Inside 4-km Domain (tpd)	Outside 4-km Domain (tpd)
Elevated Point NOx	300	4150
Low Level Point NOx	18	--
Area/Mobile/Biogenic NOx	506	8465 (incl. low level points)
Elevated Point VOC	50	860
Low Level Point VOC	220	--
Area/Mobile/Biogenic NOx	3851	67805 (incl. low level points)

Table 2-3. Summary of 2007 Strategy I8a Emission Scenarios

Scenario Name	INOx Increase (%)	IVOC Increase (%)	IOLE Increase (%)
i8a 600ole.100voc	0	0	500
80nox.600ole	100	0	500
80nox.500ole	100	0	400
80nox.400ole	100	0	300
80nox.300ole	100	0	200
80nox.200ole	100	0	100
80nox.100ole	100	0	0
80nox.00ole	100	0	-100
85nox.600ole	50	0	500
85nox.500ole	50	0	400
85nox.400ole	50	0	300
85nox.300ole	50	0	200
85nox.200ole	50	0	100
85nox.100ole	50	0	0
85nox.00ole	50	0	-100

Table 2-4 summarizes the industrial olefin and VOC emissions within the 4-km HGBPA modeling domain for both the 1993 base year and 2007 future year with adjusted (6xOLE) and unadjusted emission levels. Emissions of NOx for the 2007 I8a levels (90% reduction), the 85% and 80% reduction levels amount to 91 tpd, 126 tpd, and 162 tpd, respectively.

Table 2-4. Summary of industrial emissions for the 1993 and 2007 alternative emission scenarios (tpd).

Pollutant	1993 Base Elevated Points	1993 Base Low Level Points	1993 6 x OLE Elevated Points	1993 6 x OLE Low Level Points	2007 Ia8 Elevated Points	2007 Base Low Level Points	2007 6 x OLE Elevated Points	2007 6 x OLE Low Level Points
VOC	101	265	190.5	421	35.3	116	74.9	201
OLE	9.1	14.6	54.6	87.6	4.6	8.8	27.5	52.8
ETH	8.8	16.6	52.8	99.6	3.5	8.2	20.1	49.2

Each of the above alternative emission scenarios were simulated using Version 3.01 of the CAMx air quality model, configured as discussed above.

3. BASE YEAR MODELING RESULTS

The results of the emission sensitivity scenarios for the 1993 base year utilizing the RAMS meteorology are presented and discussed in this section.

1993 BASE YEAR MODEL PERFORMANCE EVALUATION

Version 3.01 of the CAMx air quality model was applied to the September 6-11, 1993 ozone episode using the model domain and configuration described in Section 2. The latest RAMS meteorological data fields (run r4) were used including the high-resolution 1.33-km nested grid domain. The modeling results were examined and evaluated with respect to the spatial distribution of simulated daily maximum 1-hour ozone concentrations and model performance evaluation criteria as defined by EPA guidance. A comparison with the CAMx modeling results obtained using the SAIMM meteorological fields, as well as the simulations utilizing the MM5 meteorology, was also conducted. In addition to the base year base case simulation, an enhanced industrial olefin (IOLE) emissions scenario was simulated for the 1993 base year.

Figure 3-1 displays the spatial distribution of daily maximum 1-hour ozone for the 1993 base case within the HGBPA 4-km modeling grid. The model performance statistical measures for each scenario are presented in Table 3-1, which also shows the peak modeled ozone concentration within the 4-km HGBPA domain. These data were compiled based on results at 1.33-km horizontal resolution (i.e., each 4-km grid cell contains the aggregate of 9 1.33-km cells in the area of the 1.33-km grid).

Table 3-1 displays the model performance statistical measures obtained with the RAMS meteorology as well as for both the SAIMM base case simulation and the base case simulation with the MM5 new4b simulation results for comparison. Also presented in Table 3-1 are the model performance statistics for the CAMx simulations with enhanced industrial olefin emissions. Except for the September 9th and 10th episode days, the model performance based on the RAMS meteorology meets the performance goals with respect to EPA guidance. The simulation results for the 9th and 10th of September exhibit large over-estimations of the observed ozone concentrations within the 4-km HGBPA domain.

Displays of the spatial distribution of the daily maximum 1-hour ozone concentrations are shown in the Figure 3-1 for the 1993 base case using the RAMS meteorology. The corresponding displays for the SAIMM meteorology are shown in Figure 3-2 for reference (care is needed in comparing Figures 3-1 and 3-2 because of the different color scales). An examination of Figures 3-1 and 3-2 reveal several differences between the modeling results with the SAIMM and RAMS meteorology. The spatial distribution of daily maximum ozone concentrations on September 8th show elevated ozone concentrations primarily southwest of the Houston/Galveston Bay area as well as in the Beaumont/Port Arthur region. By contrast, the SAIMM simulation results for this day produce a broad region of elevated ozone levels roughly centered over the Houston urban area and Galveston Bay. Likewise on the 9th of September, the predicted ozone peaks for the RAMS simulation occur somewhat southwest of those obtained with the SAIMM meteorology. The last day of the episode results in spatial distributions of ozone concentrations most similar to those obtained with the SAIMM, but with peak ozone levels lower than the SAIMM simulation. In general, except for the September 11th simulation day, the RAMS results exhibit much higher overall ozone concentrations throughout the 4-km modeling domain. In addition, the extent of the regions of high ozone levels tend to be greater than for the SAIMM simulations. On the 9th and 10th of September, the CAMx modeling results with the RAMS meteorology exhibit gross over-estimations of predicted daily maximum 1-hour ozone at many monitoring sites in the Houston/Galveston area. (Figure 3-3).

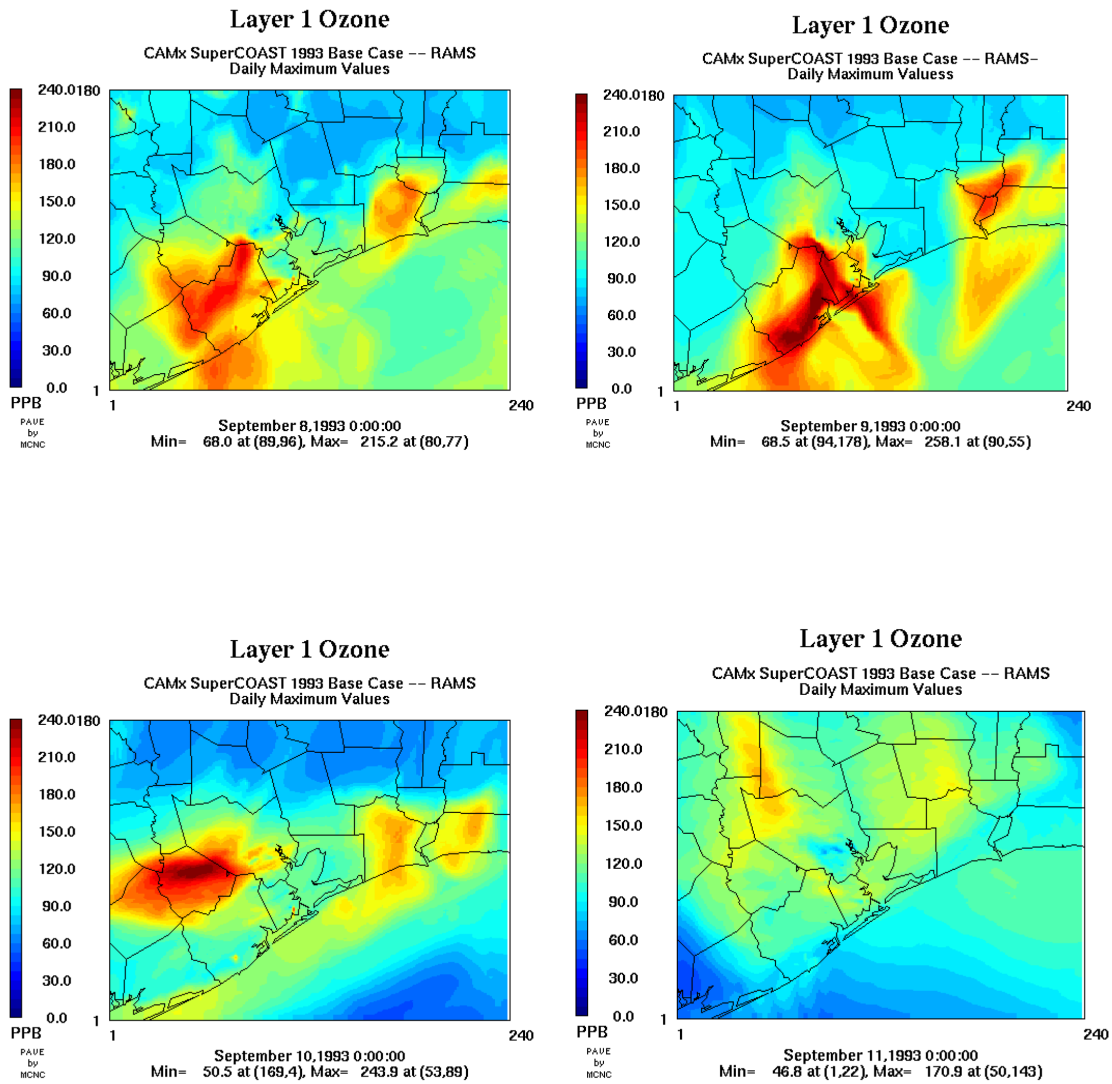

Figure 3-1. Daily maximum ozone concentrations for 1993 Base Case with RAMS meteorology (scale max = 240 ppb).

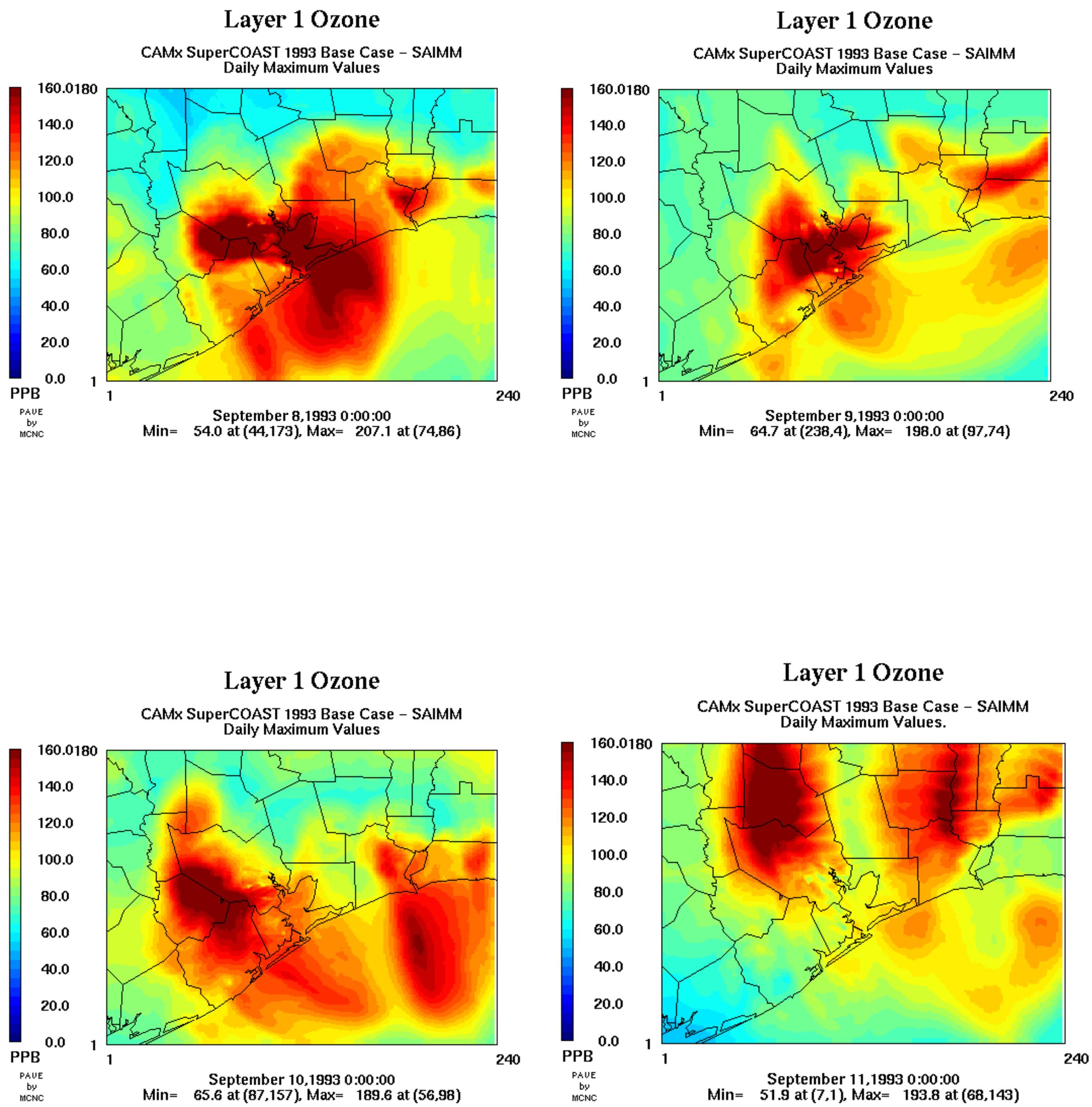

Figure 3-2. Daily Maximum ozone concentrations (ppb) on the HGBPA 4-km domain with SAIMM meteorology (scale max = 160 ppb).

Table 3-1. CAMx Model Evaluation Statistics for the 8-11 September 1993 Episode on 4-km HGBPA Domain.

Performance Attribute	**EPA Goal**	8 Sept	9 Sept	10 Sept	11 Sept
Maximum Observed Concentration (ppb)		214.0	195.0	162.0	189.0
Maximum Modeled Conc. (ppb)					
CAMx v3.01 w/ SAIMM		207.1	198.0	189.6	193.8
CAMx v3.01 w/ MM5_new4b		165.5	135.7	99.1	92.6
CAMx v3.01 w/RAMS		215.2	258.1	243.9	170.9
CAMx v3.01 w/RAMS 6xOLE		364.0	340.9	308.7	206.5
Accuracy of Unpaired Peak (%)	<"20%				
CAMx v3.01 w/ SAIMM		-3.2	1.5	17.1	2.5
CAMx v3.01 w/ MM5_new4b		-22.3	-30.4	-38.8	-51.0
CAMx v3.01 w/RAMS		0.6	32.4	50.6	-9.6
CAMx v3.01 w/RAMS 6xOLE		18.3	30.1	34.6	-6.3
Mean Normalized Bias (%)	<"15%				
CAMx v3.01 w/ SAIMM		7.1	5.3	-10.1	0.7
CAMx v3.01 w/ MM5_new4b		-10.0	-16.6	-61.9	-53.1
CAMx v3.01 w/RAMS		7.7	18.9	-7.8	-2.6
CAMx v3.01 w/RAMS 6xOLE		11.7	23.3	-1.8	1.0
Mean Normalized Gross Error (%)	<"35%				
CAMx v3.01 w/ SAIMM		25.4	27.4	25.7	21.4
CAMx v3.01 w/ MM5_new4b		17.5	23.6	62.0	53.6
CAMx v3.01 w/RAMS		32.6	39.7	41.1	21.9
CAMx v3.01 w/RAMS 6xOLE		34.7	43.0	45.0	21.4

Time series plots displayed in Figure 3-3 illustrate the 1993 base case model performance for the RAMS meteorology. In general, the model replicates the observed ozone concentration at many monitors, although on the 9^{th} and 10^{th} simulation days several sites show large over-estimation of the peak ozone concentrations.

SuperCOAST September 8-11, 1993 -- 4-km Grid

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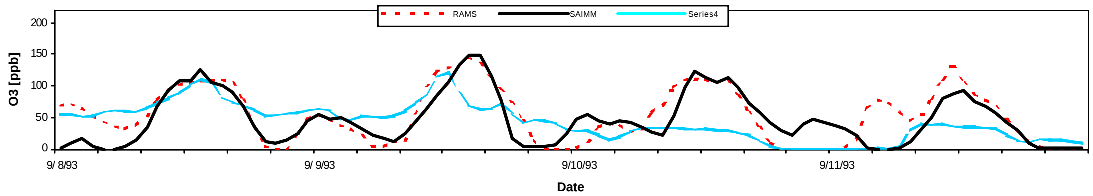
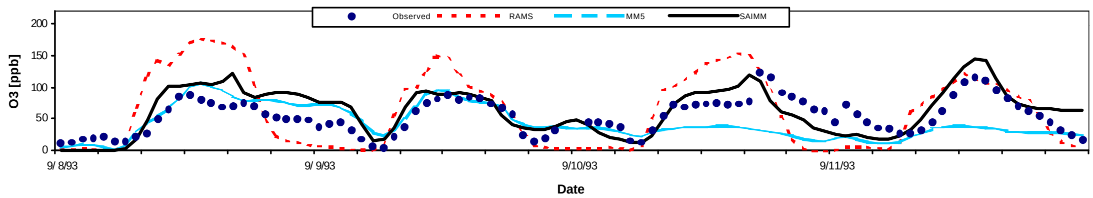
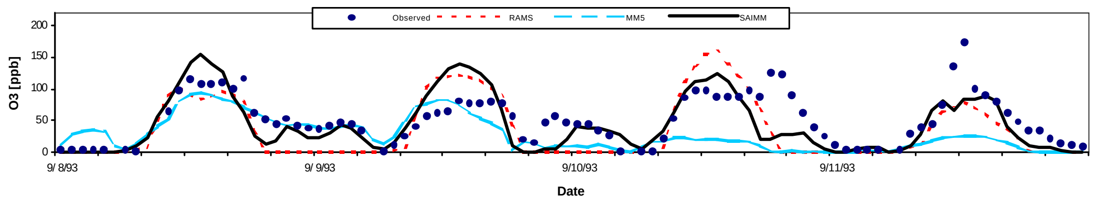


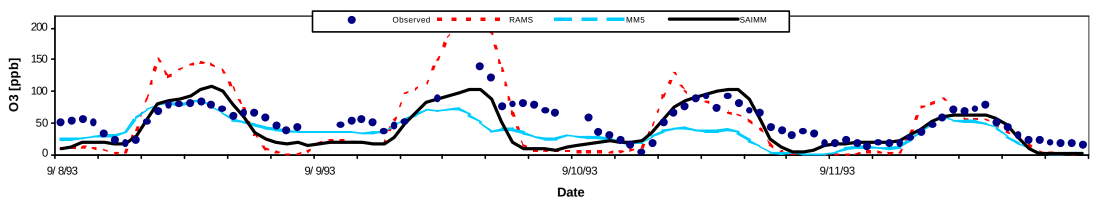
BMTC: BEAUMONT C02/JEFFERSON CO TX



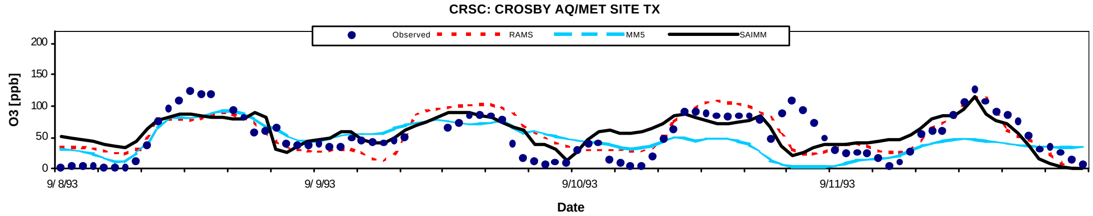
C35C: CLINTON CGC / HARRIS CO TX



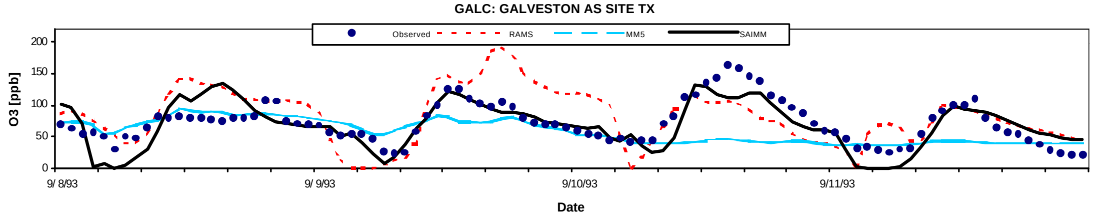
CLTA: CLUTE CAMS 11/BRAZORIA CO TX



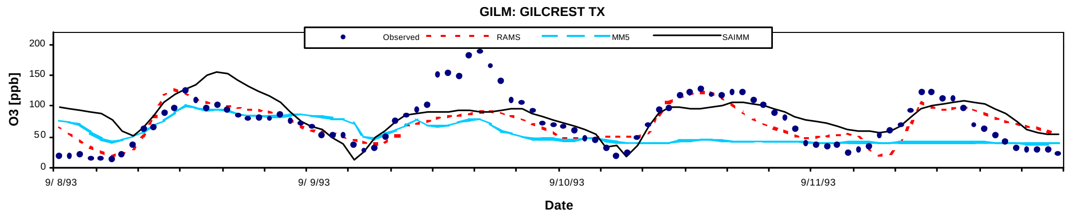
CRSC: CROSBY AQ/MET SITE TX

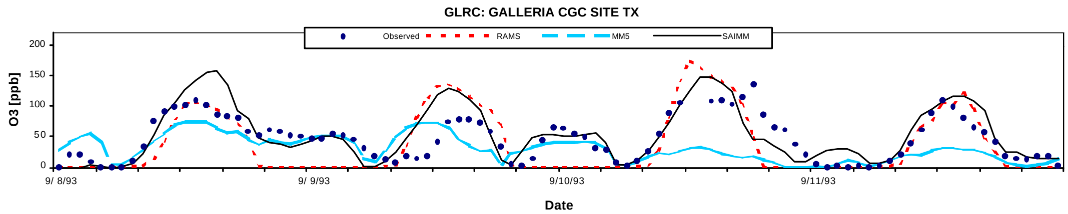


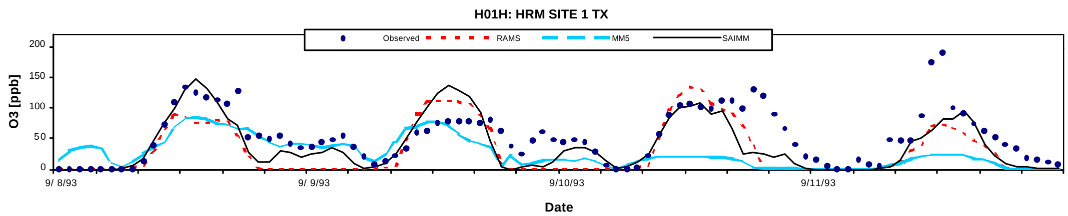
GALC: GALVESTON AS SITE TX

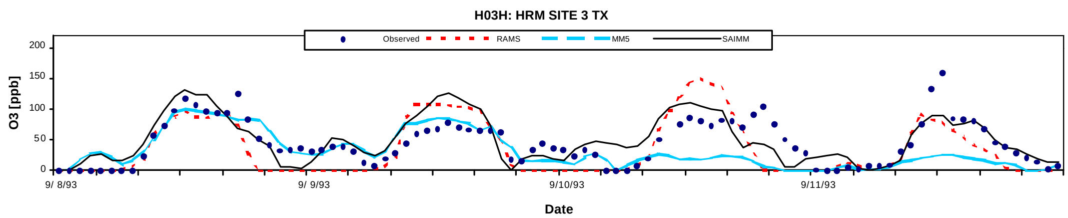


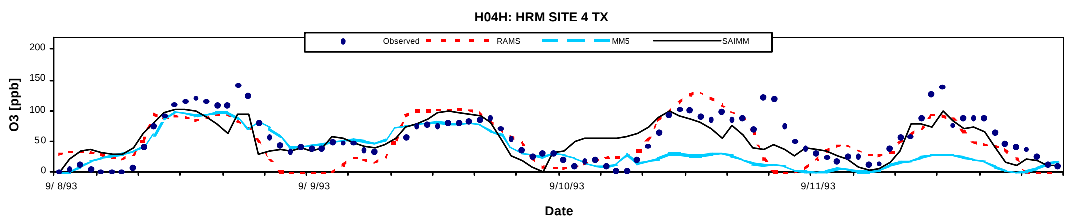
SuperCOAST September 8-11, 1993 -- 4-km Grid

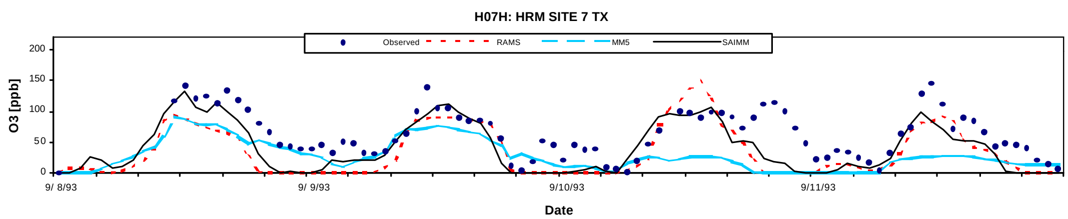












SuperCOAST September 8-11, 1993 -- 4-km Grid

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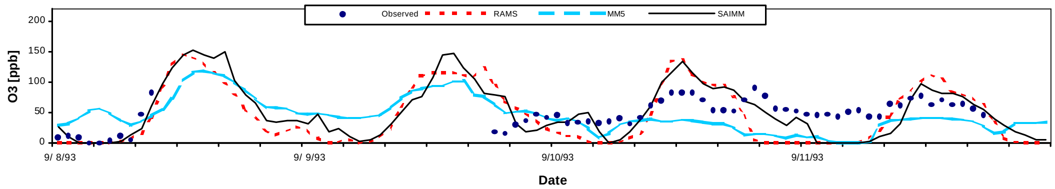

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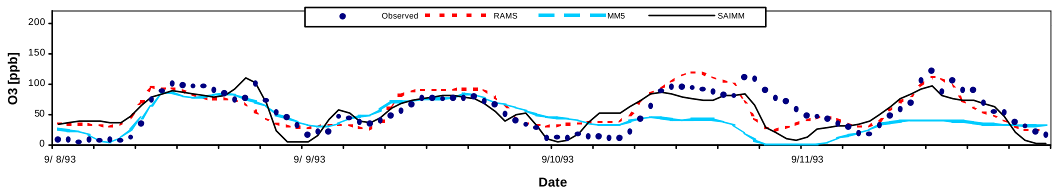

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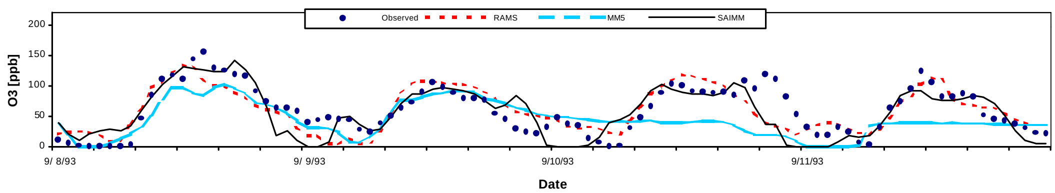
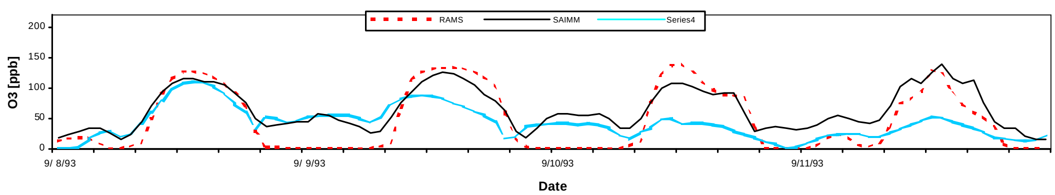
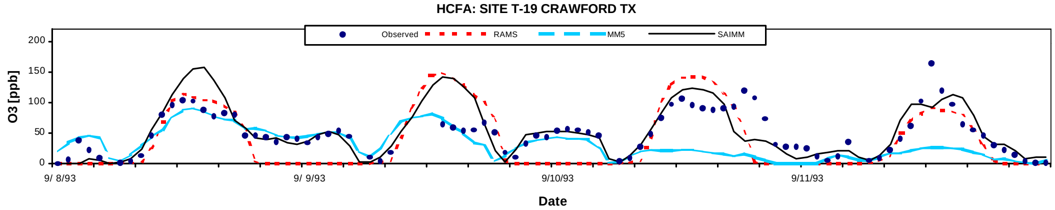


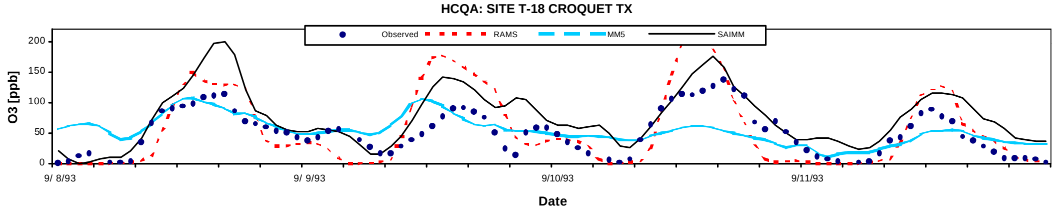
HALC: ALDINE C8/HARRIS CO TX



HCFA: SITE T-19 CRAWFORD TX

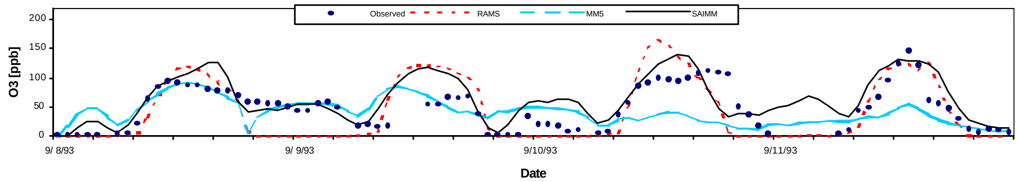


HCQA: SITE T-18 CROQUET TX

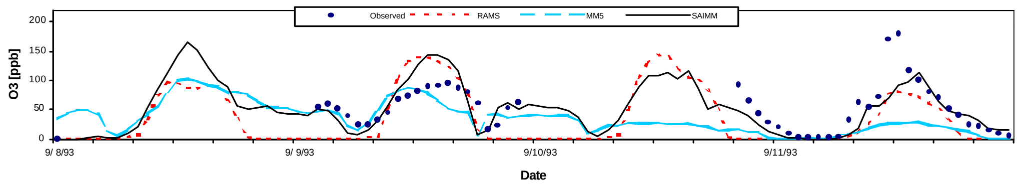


SuperCOAST September 8-11, 1993 -- 4-km Grid

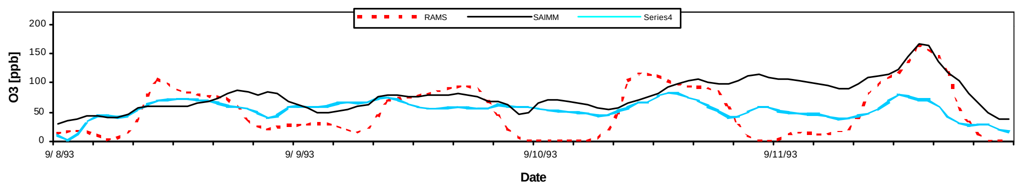
HLAA: SITE T-26 LANG TX



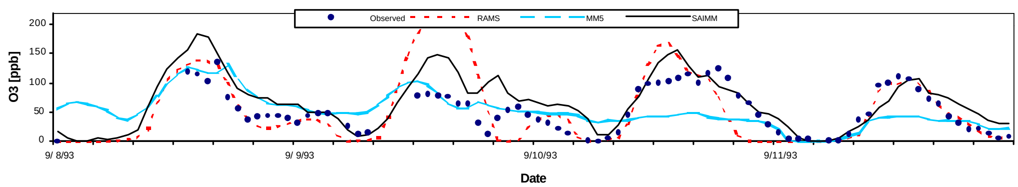
HMCA: MANCHESTER C22 TX



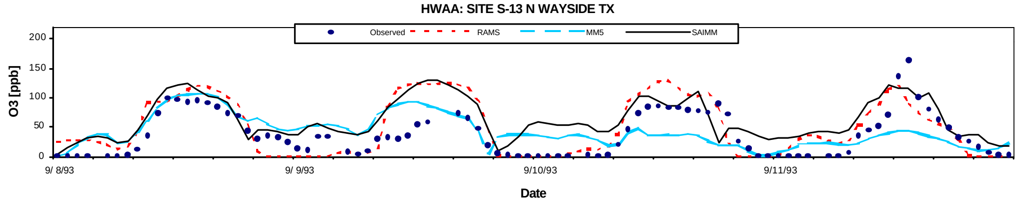
HNWA: NORTHWEST HARRIS C26 TX



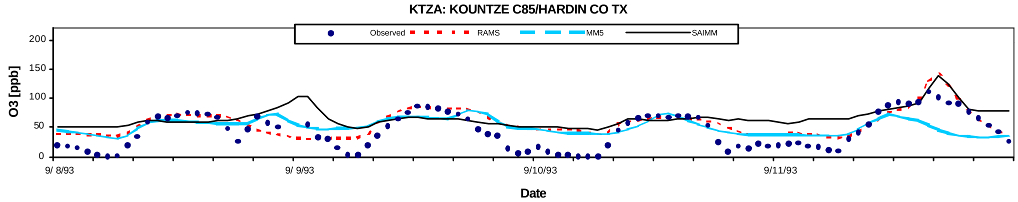
HSMA: SWISS&MONROE / HARRIS CO TX



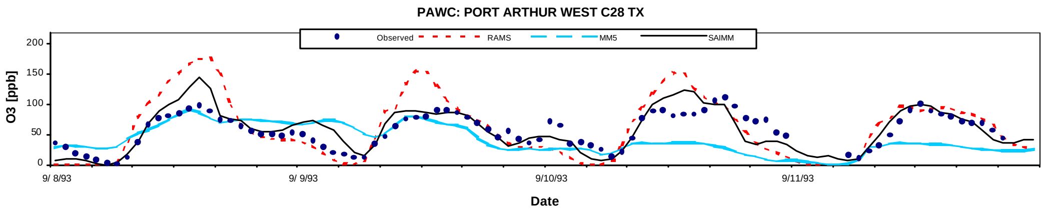
HWAA: SITE S-13 N WAYSIDE TX

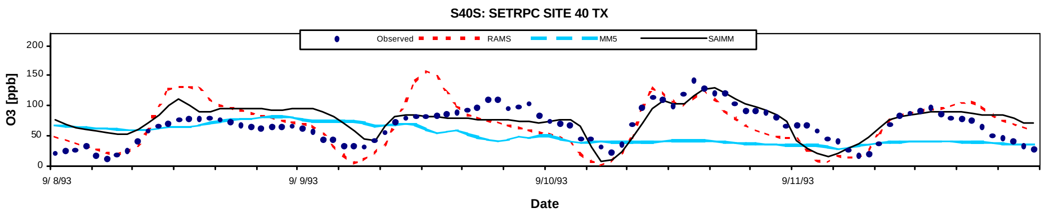


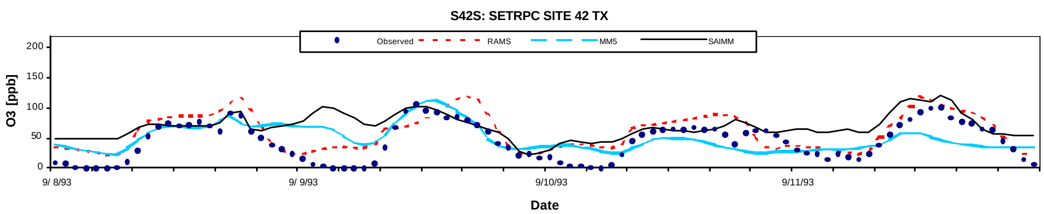
KTZA: KOUNTZE C85/HARDIN CO TX

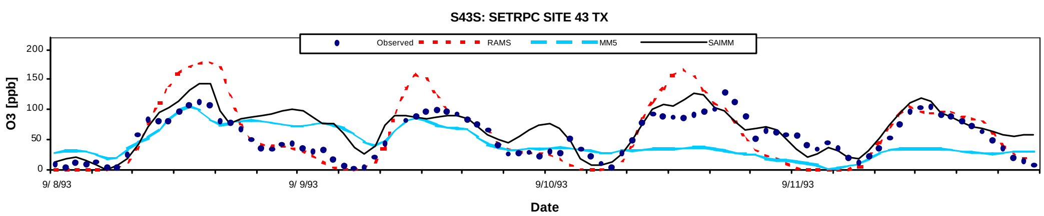


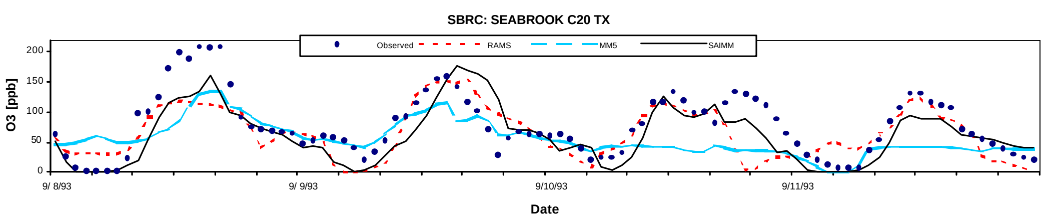
SuperCOAST September 8-11, 1993 -- 4-km Grid

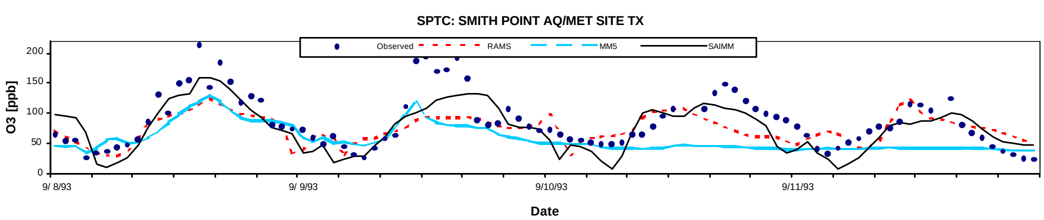






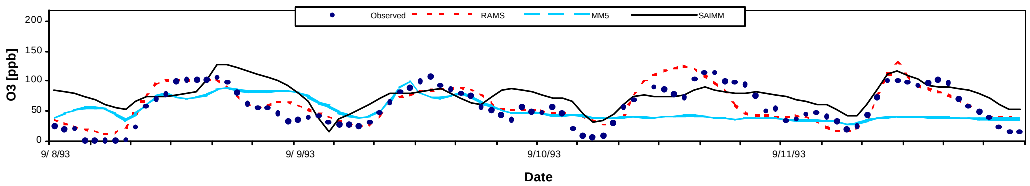




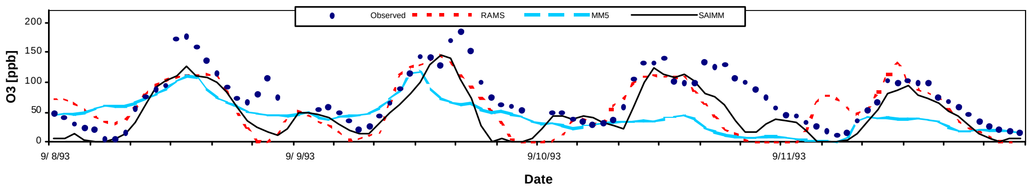


SuperCOAST September 8-11, 1993 -- 4-km Grid

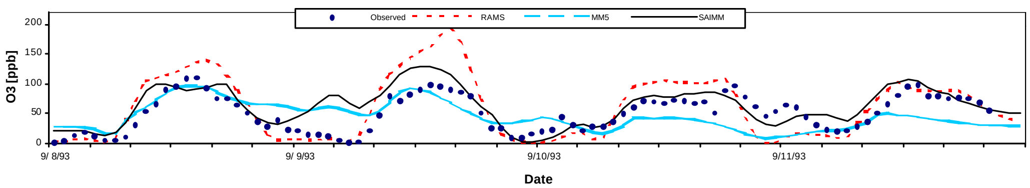
STWC: STOWELL (WINNIE) AQ/MET TX



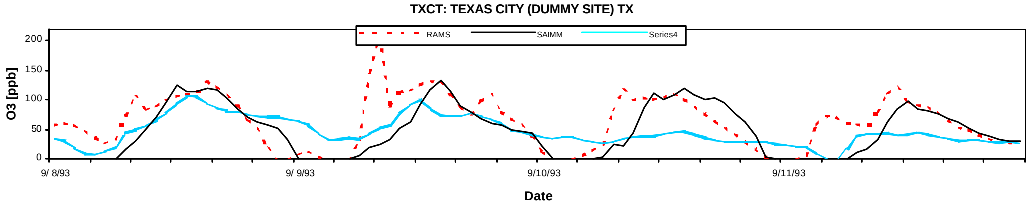
TLMC: TEXAS CITY / LA MARQUE TX



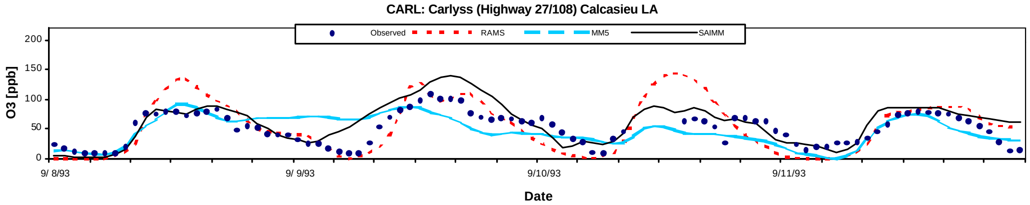
WORA: WEST ORANGE C9 TX



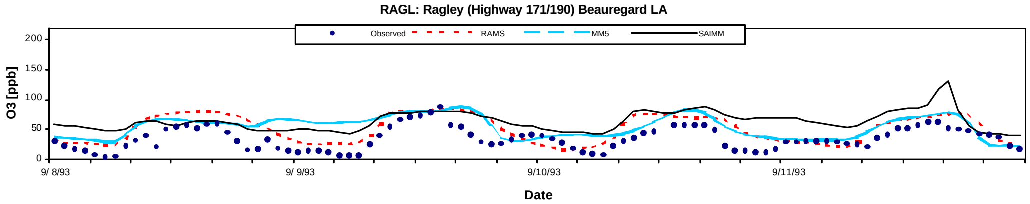
TXCT: TEXAS CITY (DUMMY SITE) TX



CARL: Carlyss (Highway 27/108) Calcasieu LA



RAGL: Ragley (Highway 171/190) Beauregard LA



SuperCOAST September 8-11, 1993 -- 4-km Grid

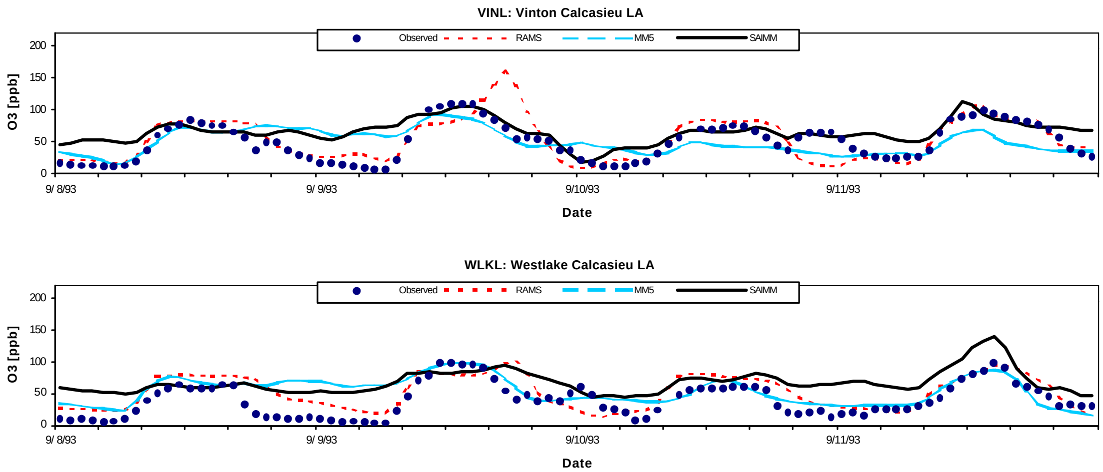


Figure 3-3. Time series plots for CAMx simulations with RAMS, MM5 and SAIMM meteorology compared to observations.

As with previous sensitivity studies of the 1993 Houston ozone episode (ENVIRON, 2002a), an emission enhancement scenario corresponding to 6x industrial olefin emissions was run. The results are presented in Figure 3-4, which displays the daily maximum 1-hour ozone concentrations within the 4-km HGBPA domain for alternative emission scenario. The resulting model performance statistics for this scenario were presented in Table 3-1. The spatial distribution of daily maximum 1-hour ozone concentrations is similar to the base case simulation although the magnitude of the predicted ozone levels are considerably higher. Comparison of the RAMS base case (Figure 3-1) and the 6xOLE case (Figure 3-4) maximum ozone for September 8th shows enhancement of several fine scale ozone plumes in the ship channel industrial area. This area is within the 1.33-km grid, and these results show that the modeling system is capable of representing fine scale ozone enhancements due to VOC releases, depending upon the meteorological fields.

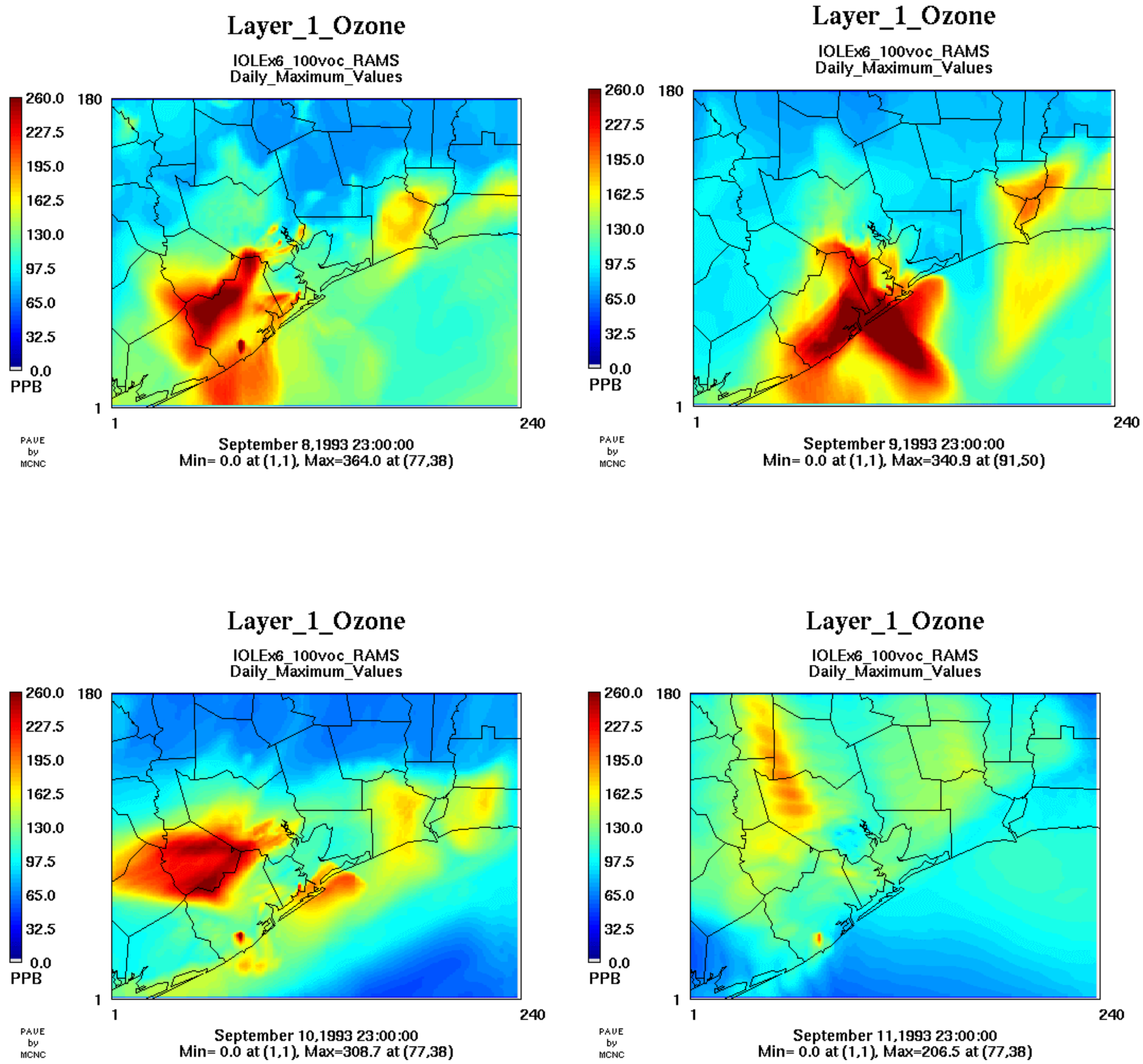


Figure 3-4. Daily maximum ozone concentrations for the 6xOLE scenario with RAMS meteorology.

The effect of increased VOC emissions on the modeled ozone concentrations was quantified through an analysis to evaluate the potential for ozone production under each emission scenario. The analysis focused on the maximum rate of ozone production from hour to hour within the 1.33-km high-resolution nested grid domain. The peak rate of ozone production was defined as the maximum difference from hour to hour of the average ozone concentrations anywhere within the 1.33-km grid. The effects of enhanced industrial VOC emissions on the ozone production rate for 1993 base year sensitivity simulation is presented in Table 3-2. These ozone production rates are seen to be considerably higher than earlier analyses of the September 1993 episode using other meteorological data fields and reflects the overall ozone over-predictions resulting from the RAMS meteorology on most days of the episode.

Table 3-2. Ozone production rates (ppb/hr) within the HGBPA domain with RAMS meteorology.

Scenario	Sept. 8, 1993	Sept. 9, 1993	Sept 10, 1993	Sept 11, 1993
Base Case	111.1	113.2	131.2	72.2
600ole.100voc	154.7	164.1	167.4	110.7

4. FUTURE YEAR MODELING RESULTS

2007 FUTURE YEAR SCENARIOS

Each of the emission scenarios developed for future year 2007were simulated using version 3.01 of the CAMx air quality model and the model domain and configuration described in Section 2. The modeling results were examined and evaluated with respect to the spatial distribution of simulated daily maximum 1-hour ozone concentrations and the impacts of each emission scenario on the daily maximum 1-hour ozone concentrations. The modeling results were also investigated to determine the necessary level of industrial olefin emission reductions required to compensate for industrial NOx emission reductions.

Based on the results of the 1993 base year modeling, and for consistency with previous analyses, the 6xOLE scenario was chosen for further analysis in the 2007 future year airquality simulations. Figure 4-1 displays the spatial distribution of daily maximum 1-hour ozone for the 6xOLE emission scenario within the HGBPA 4-km modeling grid. For this scenario, shipping emissions and new sources not subject to future year controls were taken into consideration as described previously and discussed in ENVRION, 2002b. In addition, emission adjustments were confined to the 8-county Houston-Galveston area. The daily peak 1-hour ozone concentrations in the 4-km HGBPA domain for all future year emission scenarios are presented in Table 4-1. As noted in Section 3, due to the poor model performance obtained for the first three episode days, the analyses for September 11th likely produce the only usable results.

Table 4-1. **Daily maximum ozone concentrations (ppb) for future year 2007 emission scenarios.**

Scenario Name	Sept. 8	Sept. 9	Sept. 10	Sept. 11
i8a 600ole.100voc	207.4	214.3	196.4	144.6
80nox.600ole	241.2	234.7	223.3	150.5
80nox.500ole	233.2	223.2	215.6	147.7
80nox.400ole	223.3	209.6	207.2	144.7
80nox.300ole	210.3	200.5	196.5	141.4
80nox.200ole	193.8	196.7	183.1	138.3
80nox.100ole	174.2	192.8	181.5	136.0
80nox.00ole	173.8	188.2	180.9	133.5
85nox.600ole	226.7	227.2	211.9	148.3
85nox.500ole	220.3	217.5	205.5	145.9
85nox.400ole	212.0	206.0	197.8	143.4
85nox.300ole	202.3	192.3	189.1	140.6
85nox.200ole	188.1	188.0	181.1	137.5
85nox.100ole	173.8	184.6	180.5	134.2
85nox.00ole	173.8	180.9	179.8	132.0

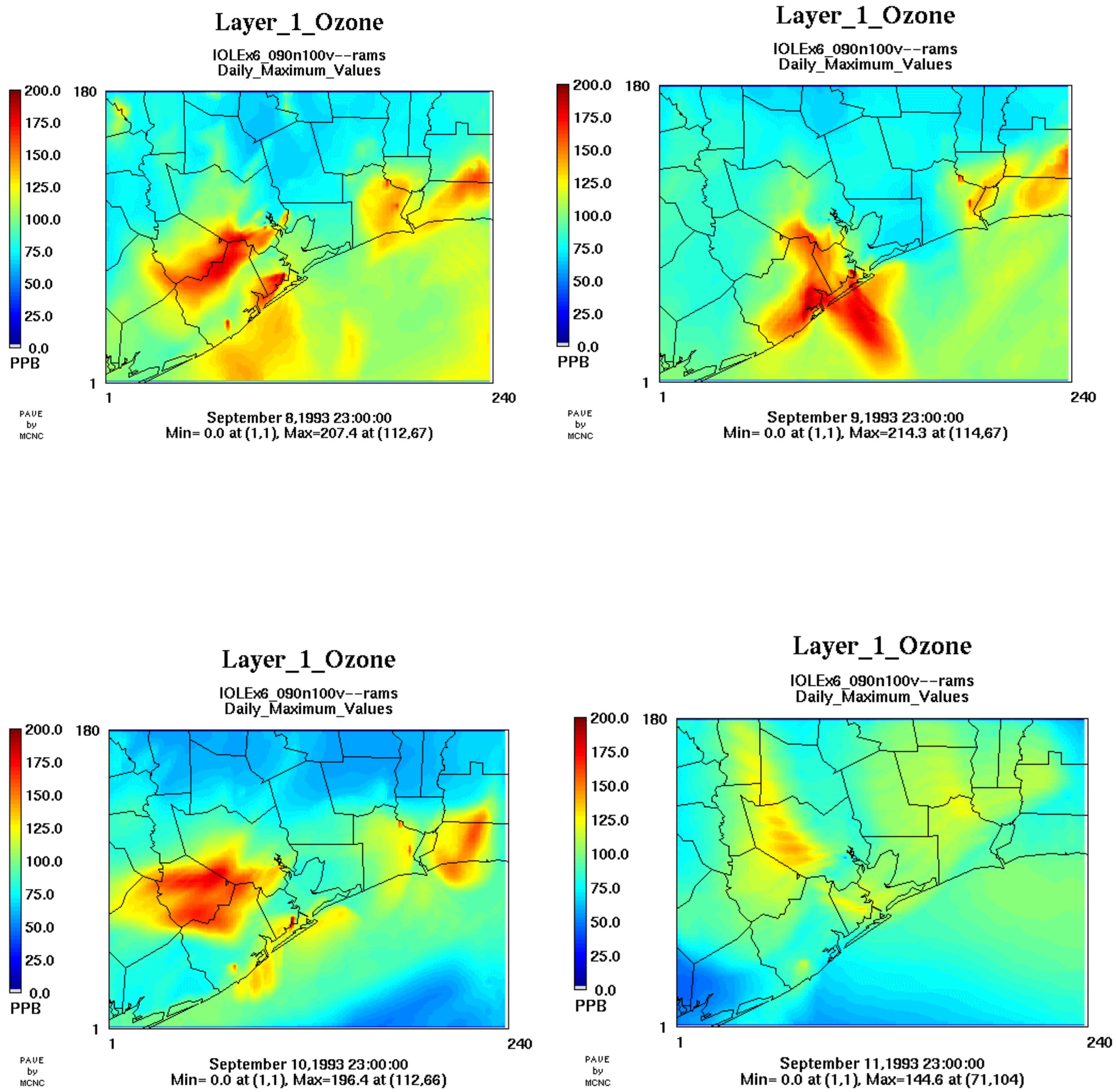


Figure 4-1. Daily maximum 1-hour ozone concentrations for the 2007 future year 6xOLE emission scenario with RAMS meteorology.

Strategy I8a includes 90% reductions in industrial NOx emissions from the 2007 base case levels. There is interest in determining whether less stringent NOx reductions (80% or 85%) could be compensated by greater reductions in 2007 industrial VOC emissions. Thus, a series of emission scenarios were conducted beginning with the 6xOLE emission level at 80% and 85% reduced NOx emission levels from the 2007 Strategy I8a scenario. After increasing the industrial NOx emission from the 2007 Strategy I8a levels, the olefin emissions were incrementally decreased to determine a compensation level of emissions required to obtain equivalent results as the 2007 Strategy I8a. The spatial distribution of daily maximum 1-hour ozone concentrations and corresponding spatial differences in daily maximum 1-hour ozone concentrations for selected olefin emission levels are displayed in Figure 4-2 through Figure 4-7 for the 80% industrial NOx emission levels. Figures 4-8 through Figure 4-10 display the difference isopleths for the modeling results at the 85% industrial NOx reduction level.

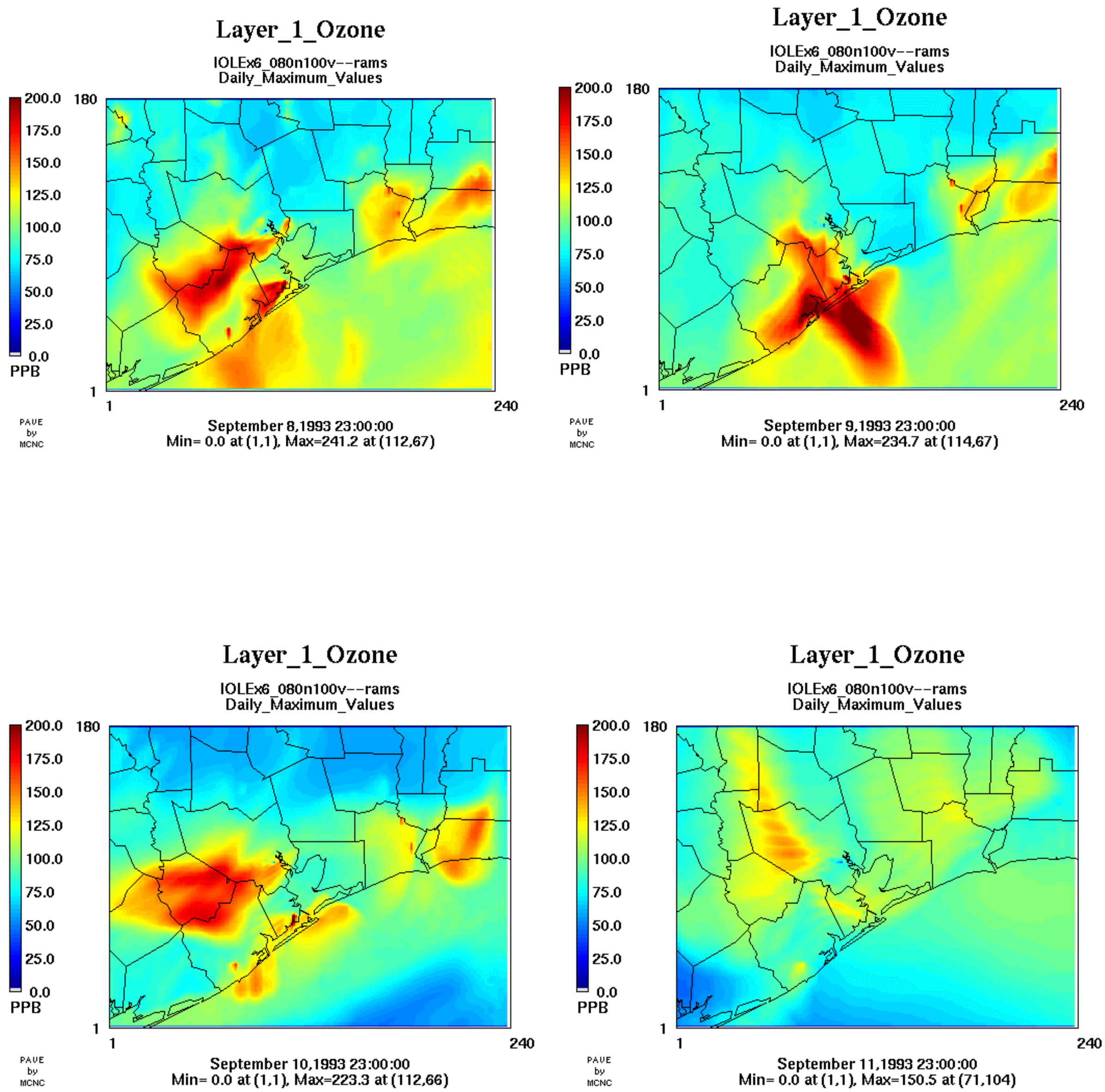


Figure 4-2. Daily maximum ozone concentrations for future year 2007 at 6x industrial olefins and double Strategy I8a NOx emission levels (80% reduction).

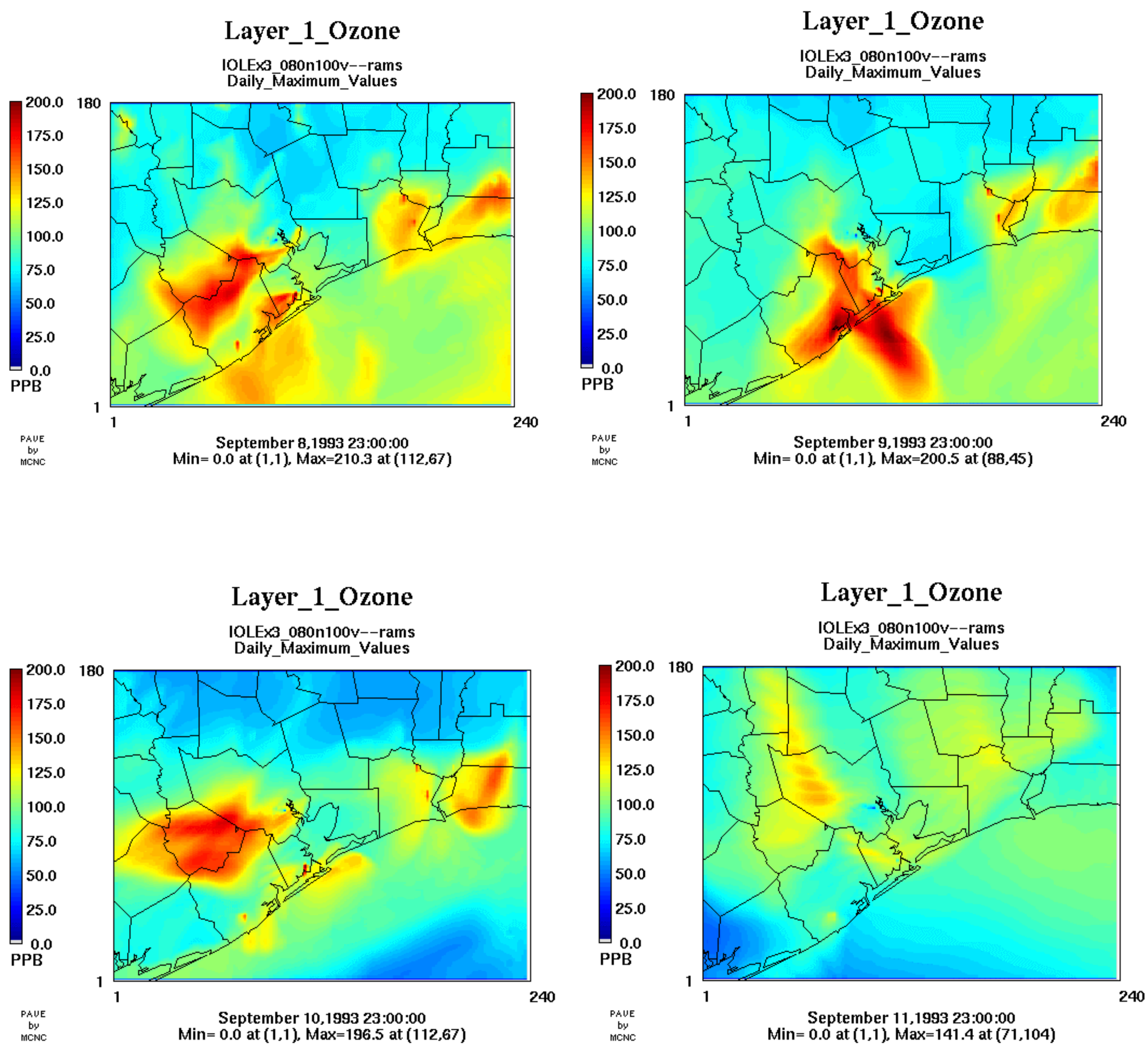


Figure 4-3. Daily maximum ozone concentrations for future year 2007 at 3x industrial olefins and double Strategy I8a NOx emission levels (80% reduction).

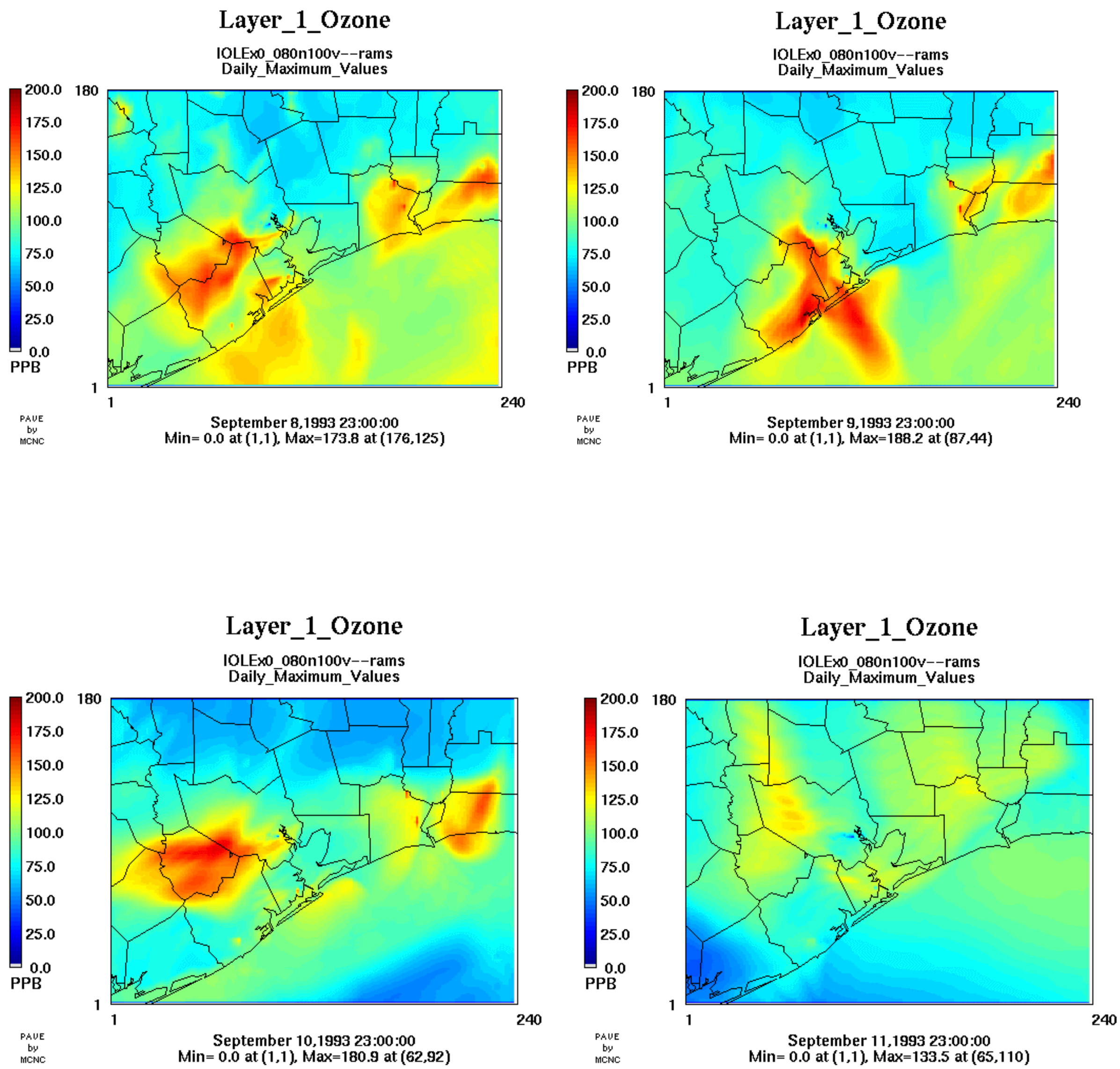


Figure 4-4. Daily maximum ozone concentrations for future year 2007 with zero industrial olefin emissions and double Strategy I8a NOx emission levels (80% reduction).

Figure 4-5 illustrates the effects of “doubled” industrial NOx emissions on the 2007 future year simulation results with 6xOLE emissions levels. Increasing NOx emissions within the 8-county region results in increased ozone concentrations throughout the Houston/Galveston Bay area. On the September 8th simulation day, the ozone increases are slightly southwest of the Houston urban area and extend offshore. The results for the 9th of September display regions of increased ozone levels within the ship channel and Galveston Bay area. Localized ozone decreases are also evident within the Houston area. Similar results are seen on the remaining days of the episode. The effects of “doubled” industrial NOx and a 50% decrease in industrial olefin emissions are displayed in Figure 4-6. On all episode days, regions of ozone decreases are realized within and downwind of Houston and Galveston Bay while smaller regions of ozone increases are still present. The reduction in ozone concentrations under this scenario range from approximately 22 ppb on the 11th to 52 ppb on the 8th of September. Figure 4-7 illustrates the effect of doubled industrial NOx and 100% reduction in industrial olefin emissions. This case represents the maximum potential ozone reductions achievable for this alternative emission scenario. As in the case of 50% decrease in industrial olefin emissions, regions of ozone increases and decreases are seen. The ozone decreases for this case appear to cover more broad regions with fewer and smaller ozone increases being realized. Ozone reductions for this case range from approximately 37 ppb on the 11th to 72 ppb on September 8th. Comparing these results with those obtained with the SAIMM simulations shows much larger regions of decreases in ozone concentrations and the magnitudes of the ozone reductions are higher. Results for the 85% industrial NOx emission reduction level are similar with respect to the spatial distributions although the magnitude of possible ozone reductions is slightly larger.

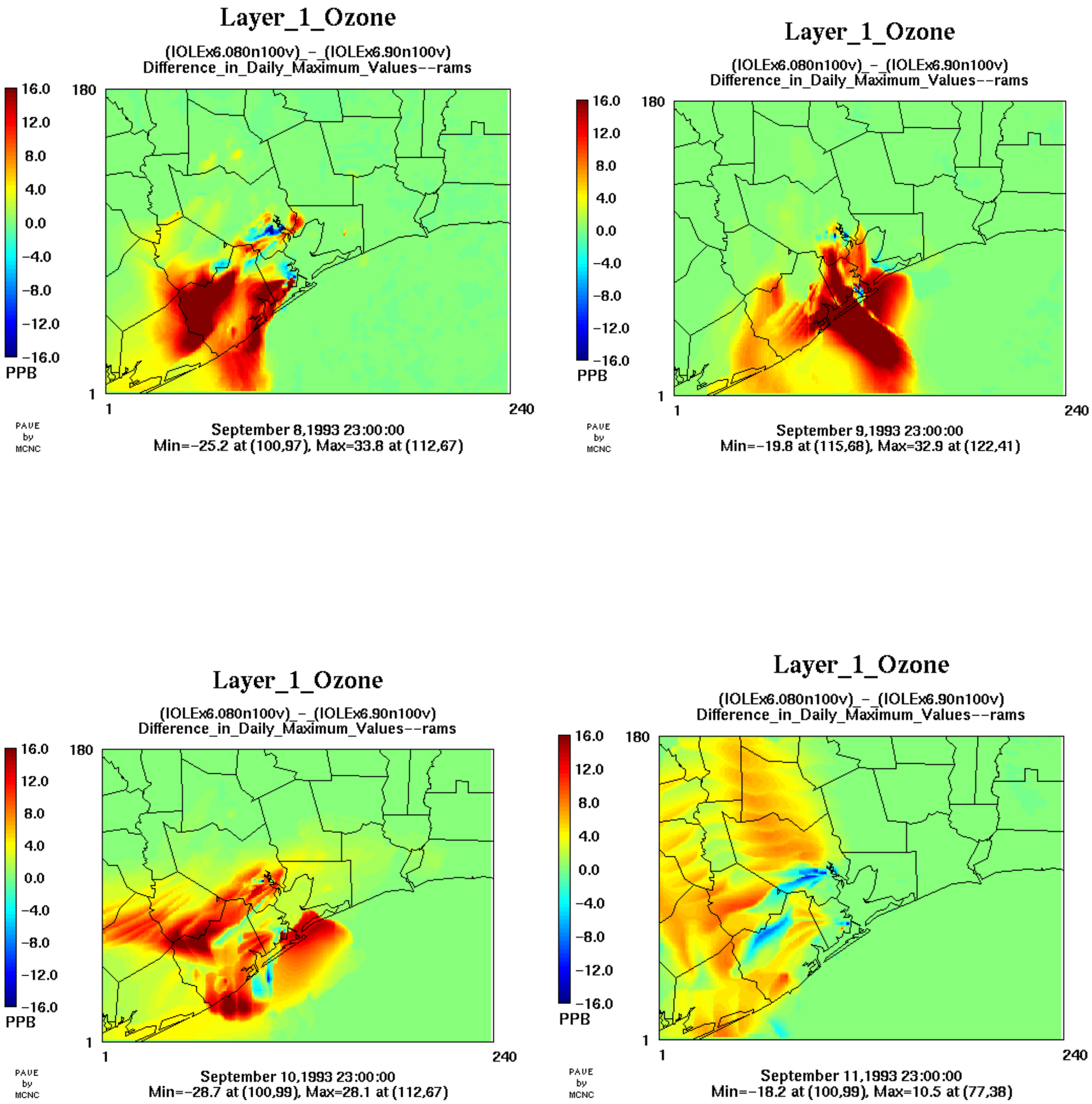


Figure 4-5. Effects of doubled industrial NOx emissions on daily maximum ozone concentrations for future year 2007.

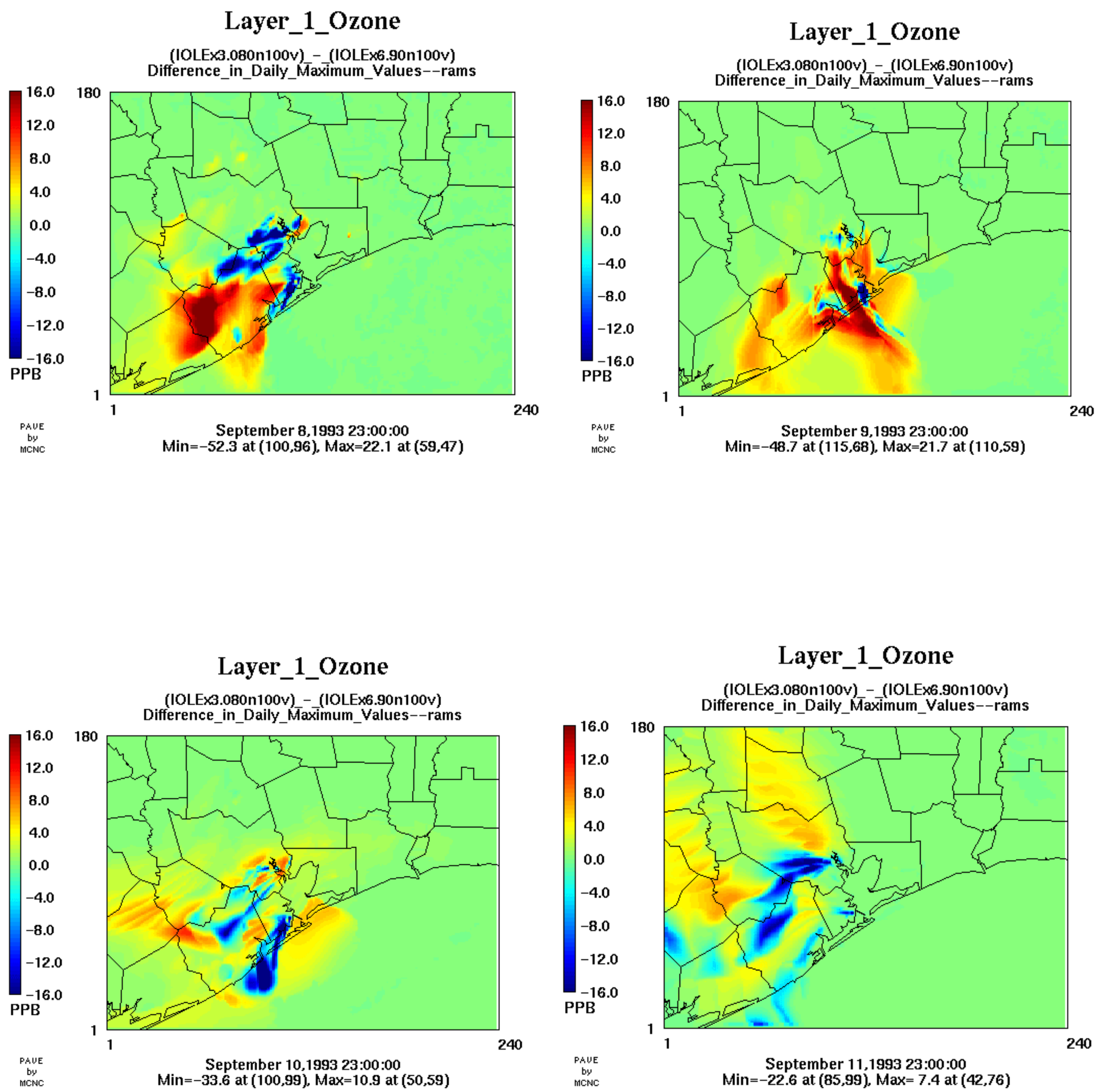


Figure 4-6. Effects of doubled industrial NOx emissions and 50% reduction of industrial olefin emissions on daily maximum ozone concentrations for future year 2007.

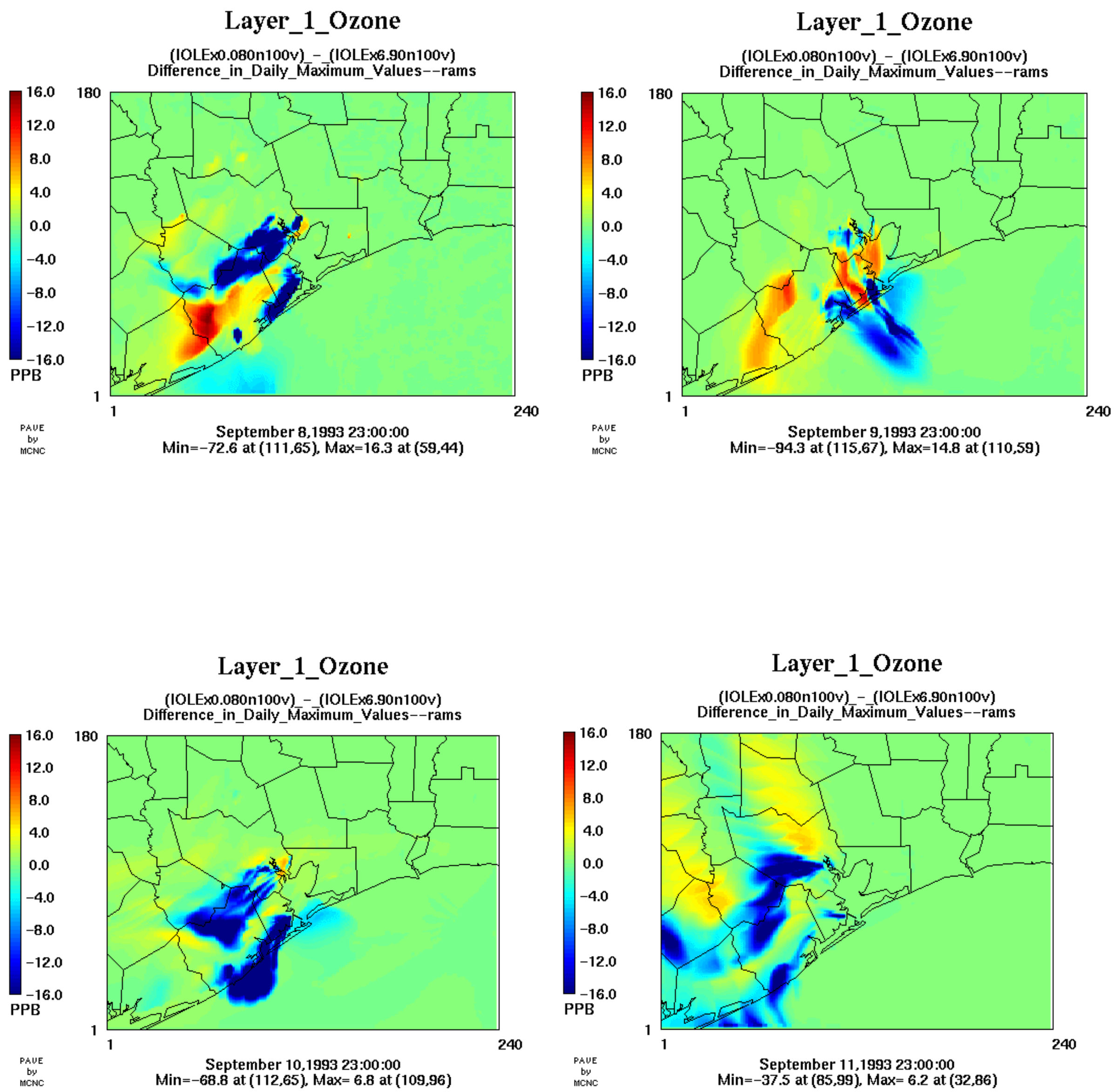


Figure 4-7. Maximum potential ozone reductions from the doubled Strategy i8a NOx emission levels (80% reduction) resulting from 100% reduction of industrial olefin emissions.

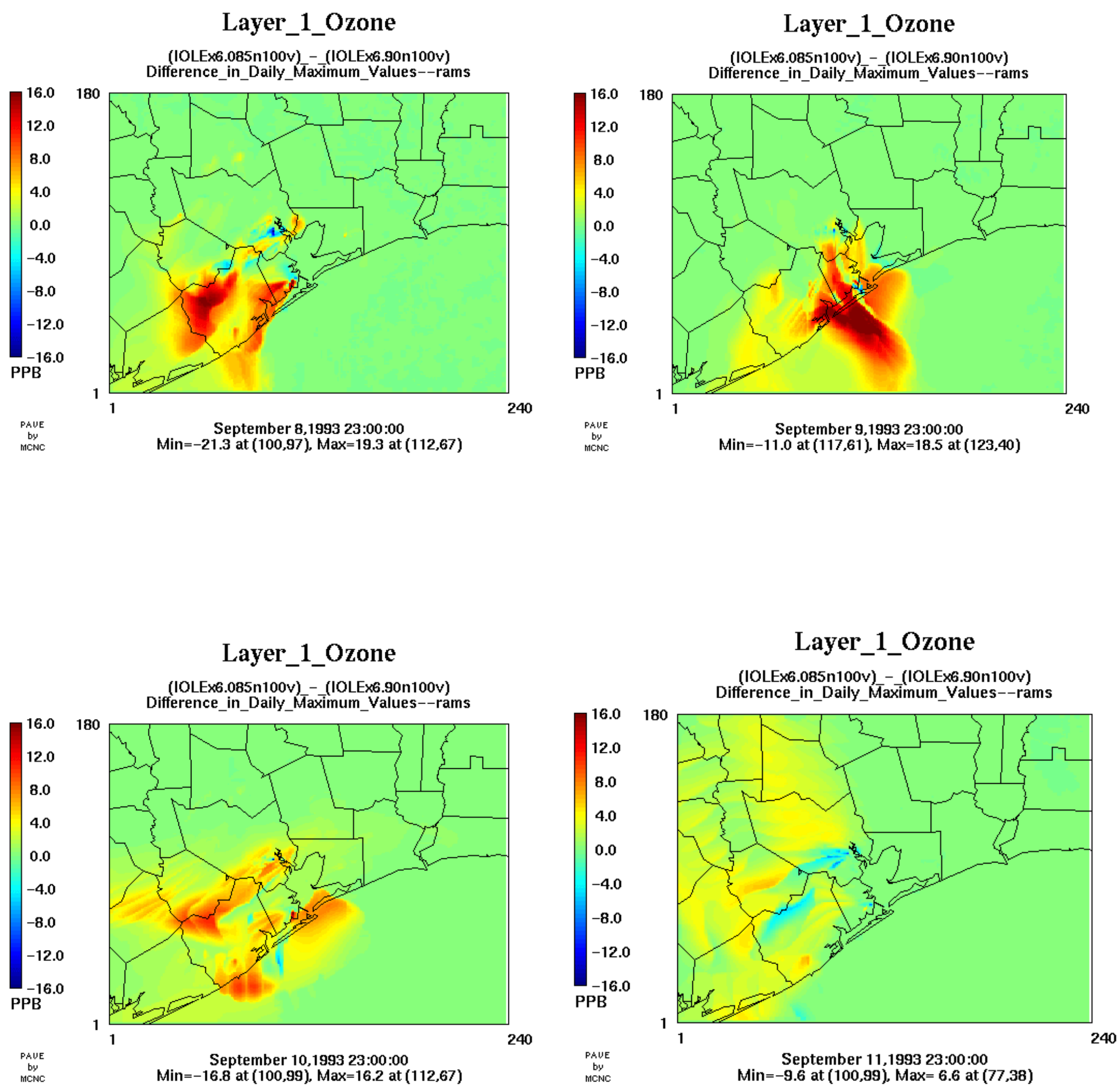


Figure 4-8. Effects of 150% industrial NOx emissions on daily maximum ozone concentrations for future year 2007.

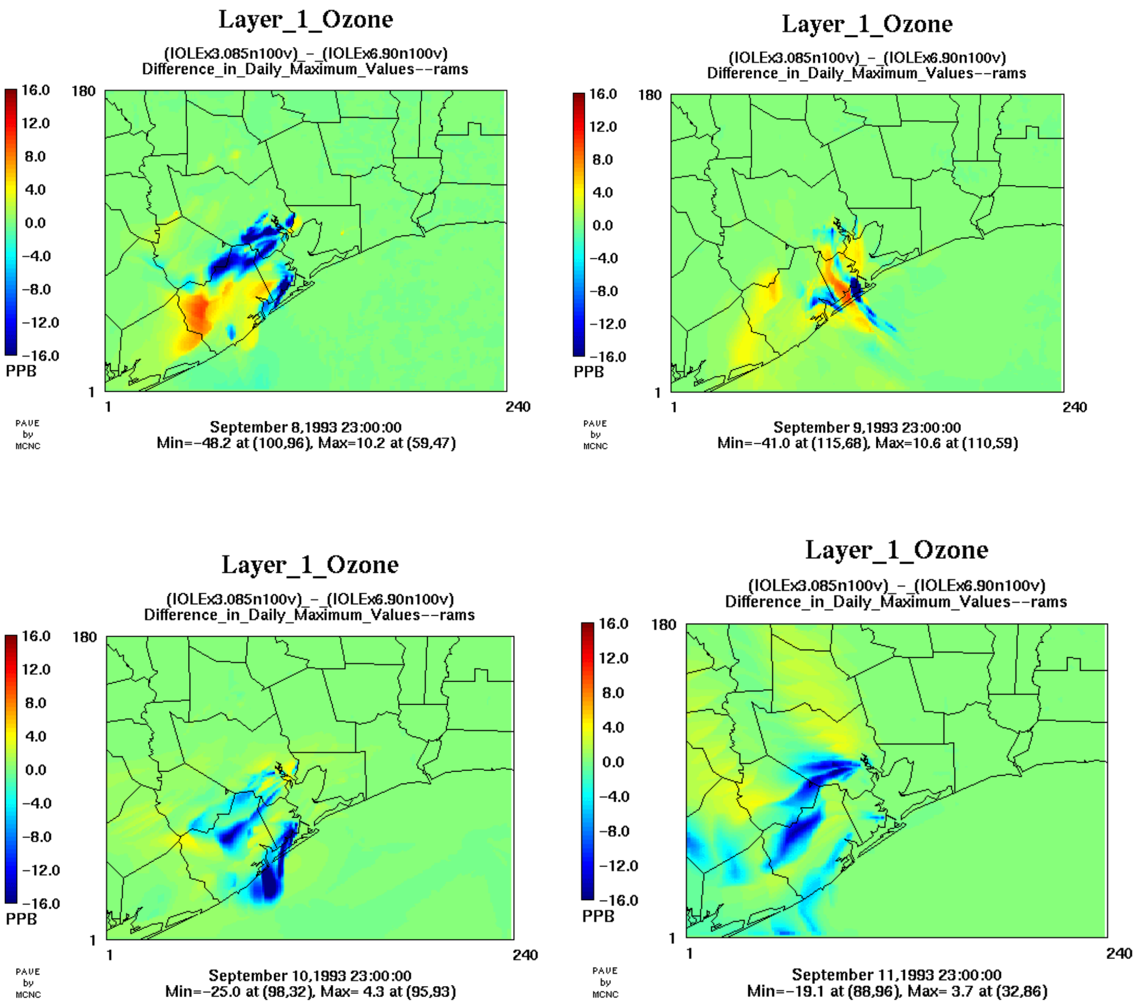


Figure 4-9. Effects of 150% industrial NOx emissions and 50% reduction of industrial olefin emissions on daily maximum ozone concentrations for future year 2007.

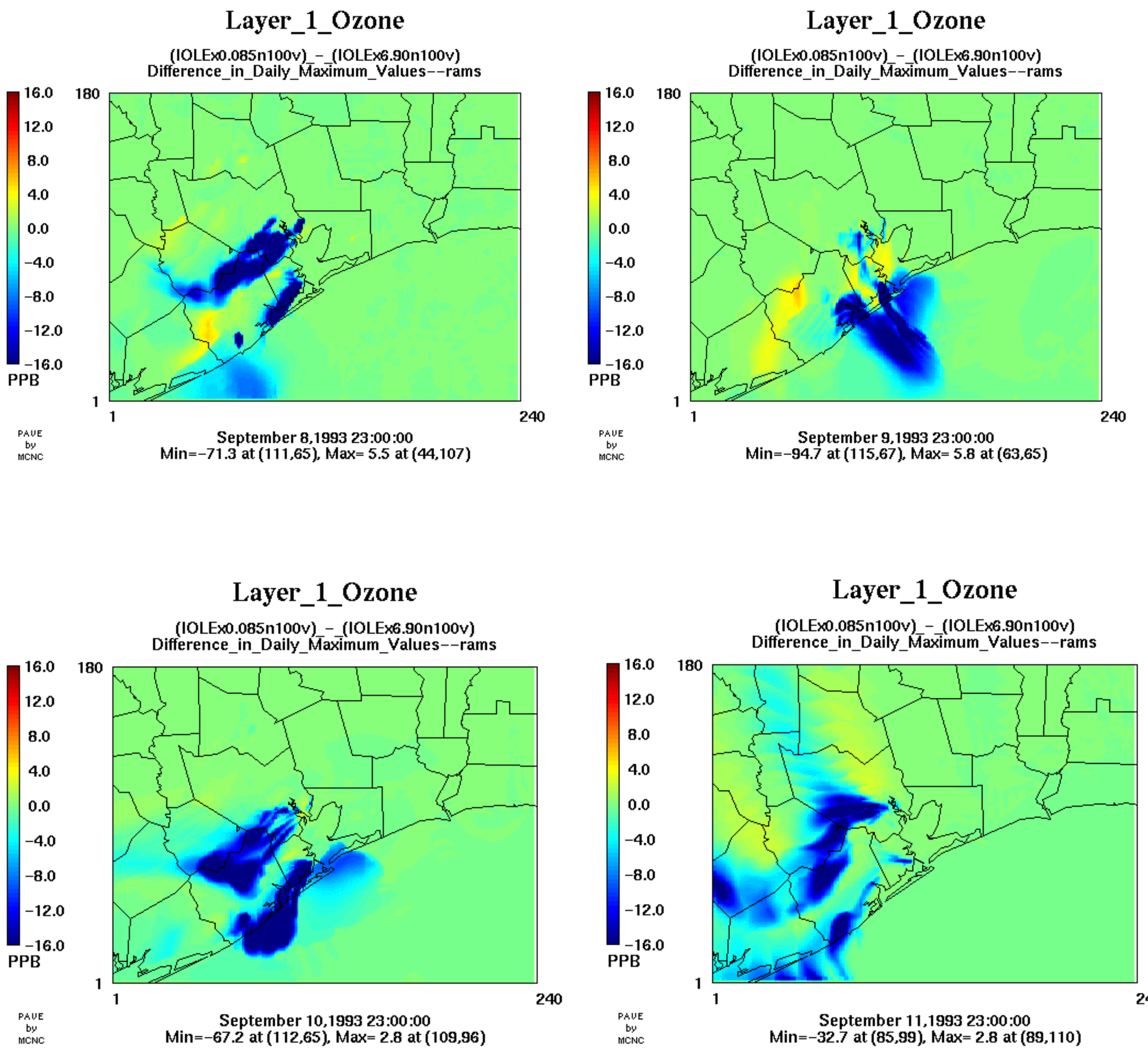


Figure 4-10. Maximum potential ozone reductions from the 150% Strategy i8a NOx emission levels (85% reduction) resulting from 100% reduction of industrial olefin emissions.

Tables 4-2 and 4-3 present a quantitative analysis of the sensitivity scenarios investigated in this study. In Tables 4-2 and 4-3 the 90nox.600ole simulation represents the peak ozone concentration value which must be matched through reductions in industrial olefin (IOLE) emission levels. The 80nox.600ole simulation values provide the starting point for olefin emission reductions. The highlighted values in the Tables give the closest match obtained for the reduction scenarios considered. The necessary levels of olefin emission reductions required to compensate for industrial NOx emission reductions are seen to depend on the episode day.

As an example, on the September 11th episode day, doubling the industrial NOx emissions increases the peak ozone concentration in the 4-km HGBPA domain to 148.3 ppb. Subsequent reduction of IOLE emission levels to zero brings the peak ozone level down to 134.2 ppb. At the 4xOLE emission level, the peak on the 11th is approximately 143.4 ppb. Therefore, for this day, NOx emission reductions in the future year control case can be compensated for with an approximately 30% reduction in industrial olefin emissions. The analyses for the other episode days are similar, resulting in the following compensation levels: ~60% on September 8th; ~25% on September 9th; ~70% on September 10th; and ~30% on September 11th.

Table 4-2. INOx/IOLE Equivalence at the 80% NOx emissions level.

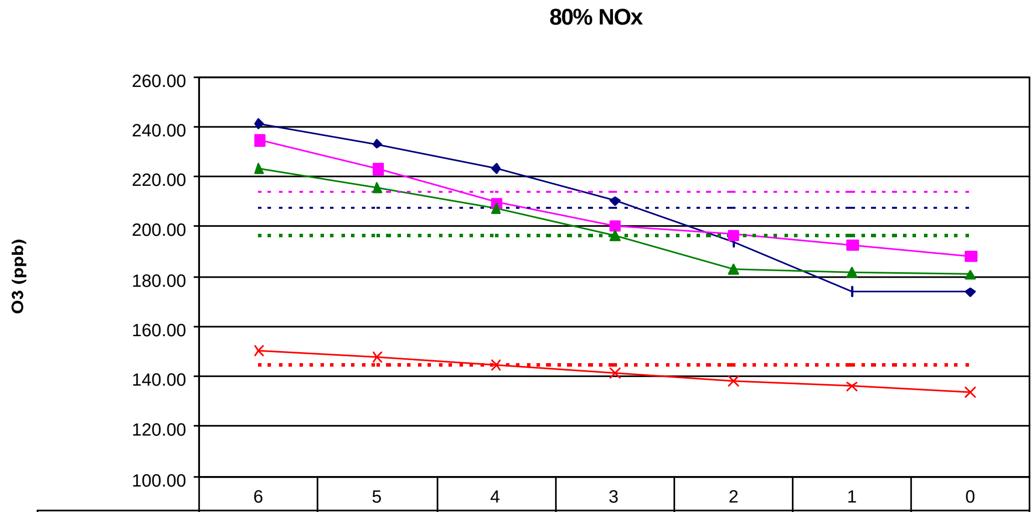
Date/ Time	90nox 6ole	80nox 6ole	80nox 5ole	80nox 4ole	80nox 3ole	80nox 2ole	80nox 1ole	80nox 0ole
9/8 Max	207.4	241.2	233.2	223.3	210.3	193.8	174.2	173.2
9/9 Max	214.3	234.7	223.2	209.6	200.5	196.7	192.8	188.2
9/10 Max	196.4	223.2	215.6	207.2	196.5	183.1	181.5	180.9
9/11 Max	144.6	150.5	147.7	144.7	141.4	138.3	136.0	133.5

Repeating the analysis for the 85% NOx emission level scenarios gives the following IOLE emission reductions necessary for each day: ~40% on September 8th; ~80% on September 9th; ~70% on September 10th; and ~25% on September 11th.

Table 4-3. INOx/IOLE Equivalence at the 85% NOx emissions level.

Date/ Time	90nox 6ole	85nox 6ole	85nox 5ole	85nox 4ole	85nox 3ole	85nox 2ole	85nox 1ole	85nox 0ole
9/8 Max	207.4	226.7	220.3	212.0	202.3	188.1	173.8	173.8
9/9 Max	214.3	227.2	217.5	206.0	192.3	188.0	184.6	180.9
9/10 Max	196.4	211.9	205.5	197.8	189.1	181.1	180.5	179.8
9/11 Max	144.6	148.3	145.9	143.4	140.6	137.5	134.2	132.0

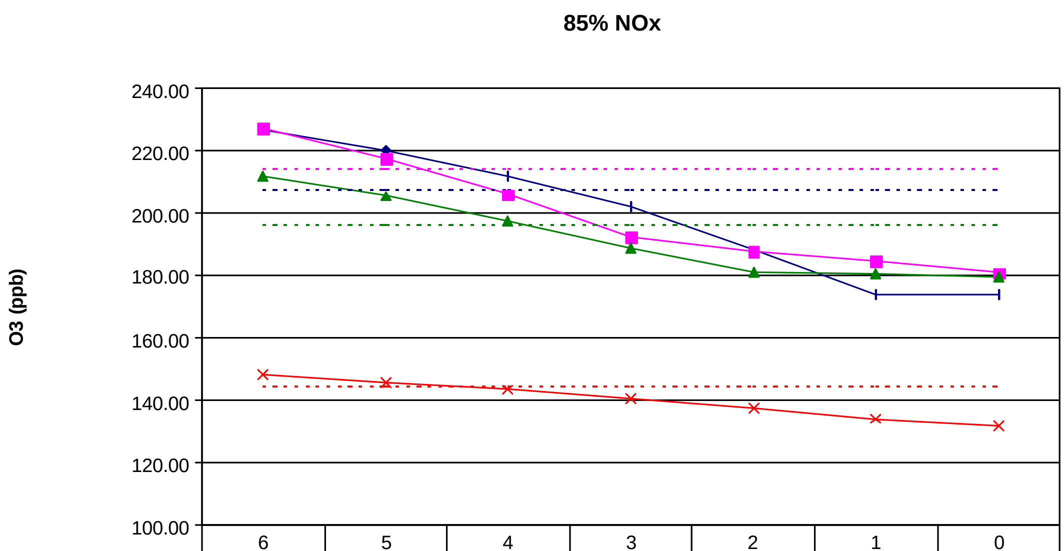
Figure 4-11 and 4-12 display these relations graphically and provide a means for interpolating the results to other industrial olefin emission reduction levels that lie between the levels modeled. These figures display the modeled peak ozone concentration as a function of the industrial olefin emission reduction levels for each day of the simulation. Also shown are the target peak ozone levels, i.e., the peak ozone concentrations resulting from the model simulations with 90% NOx emission reduction and 6xIOLE emissions. The intersection of the curves gives the required level of IOLE emission reductions to compensate for the increased industrial NOx emission reductions for each day of the episode. The response of the modeled ozone peaks due to industrial olefin emission reductions can be seen to depend on the episode day.



OLE	6	5	4	3	2	1	0
8-Sep	241.20	233.15	223.32	210.25	193.75	174.20	173.76
9-Sep	234.74	223.18	209.60	200.49	196.72	192.75	188.22
10-Sep	223.33	215.63	207.23	196.51	183.10	181.47	180.86
11-Sep	150.49	147.73	144.69	141.35	138.32	135.99	133.52
9/8 Target	207.43	207.43	207.43	207.43	207.43	207.43	207.43
9/9 Target	214.30	214.30	214.30	214.30	214.30	214.30	214.30
9/10 Target	196.41	196.41	196.41	196.41	196.41	196.41	196.41
9/11 Target	144.62	144.62	144.62	144.62	144.62	144.62	144.62

OLE

Figure 4-11. Graphical representation of INOx/IOLE equivalency for the 80% INOx series.



OLE	6	5	4	3	2	1	0
8-Sep	226.69	220.34	212.09	202.03	188.10	173.76	173.76
9-Sep	227.21	217.49	205.99	192.30	187.98	184.56	180.89
10-Sep	211.89	205.49	197.76	189.05	181.13	180.45	179.75
11-Sep	148.30	145.96	143.44	140.64	137.54	134.22	132.00
9/8 Target	207.43	207.43	207.43	207.43	207.43	207.43	207.43
9/9 Target	214.30	214.30	214.30	214.30	214.30	214.30	214.30
9/10 Target	196.41	196.41	196.41	196.41	196.41	196.41	196.41
9/11 Target	144.62	144.62	144.62	144.62	144.62	144.62	144.62

OLE

Figure 4-12. Graphical representation of INOx/IOLE equivalency for the 85% INOx series.

5. SUMMARY

The CAMx air quality model was applied to the September 8-11, 1993 ozone episode on the SuperCOAST domain. High resolution RAMS meteorological fields developed by Tremback and Emery (2001) were used with version 3.01 of the CAMx model including chlorine chemistry. A high resolution 1.33-km nested modeling grid over the Houston Ship Channel and Galveston Bay was included. As documented previously (ENVIRON, 2002), this model version and configuration provided acceptable model performance on August 8th and 11th, 1993. The response of the model to emission scenarios used by the TNRCC for control strategy evaluation was determined to be consistent with the response obtained using the same model version (2.03) and configuration as used in the development of the December 2000 SIP.

Emission sensitivity simulations were conducted to assess model performance under various alternative emission scenarios selected to reflect a more realistic estimate of VOC emission levels consistent with the 2000 TexAQS analysis.

Future year 2007 control simulations were conducted under various alternative industrial VOC emission scenarios. Industrial VOC emission adjustments were developed within an 8-county Houston-Galveston region with appropriate consideration given for sources not subject to future year controls. A series of future year emission scenarios were conducted to evaluate the potential of alternative VOC emission reductions to compensate for NOx emission reductions currently implemented in the future year 2007 Strategy i8a SIP simulations.

A number of summary conclusions can be drawn from the model simulations performed for this study:

- The RAMS-based simulations included high-resolution 1.33-km meteorology within the Galveston Bay area and thus no flexi-nesting features were required for the meteorology. However, the area source emissions data was still interpolated to the 1.33-km fine grid modeling domain.

- The resulting model performance was acceptable at many monitoring sites on the 8th and 11th of September, although there was a tendency to over-predict the highest ozone levels in the Galveston Bay area. Very poor model performance was achieved on the 9th and 10th of September. Investigating the reasons for poor model performance on the 9th and 10th was outside the scope of this work.

- Increasing olefin emissions from industrial sources increased predicted ozone levels in the Galveston Bay area on September 8th, 9th and 10th, degrading the model performance. Based on the ozone performance for the September 11th episode day, and for consistency with previous similar sensitivity analyses using other meteorology, the 6xOLE emission scenario was selected for further analysis and evaluation.

- Comparison of the predicted daily maximum 1-hour ozone concentrations for the RAMS base and the 6xOLE case for many episode days shows enhancement of several fine scale ozone plumes in the ship channel industrial area. As this area is within the 1.33-km grid, these results illustrate the capability of the high resolution CAMx modeling system to represent fine scale ozone enhancements due to VOC releases, depending upon the meteorological fields. The peak ozone production rates were also substantially accelerated by increasing the industrial olefin emissions on all days, with rates as high as 167 ppb/hr modeled.

- An analysis of the alternative emission scenarios for the future year control case demonstrate the response of the modeling system to varying industrial NOx and VOC control strategies. Model response is shown to vary depending on the episode day. The potential for compensating NOx emission reductions with appropriate industrial olefin (IOLE) emission reductions has been shown to be theoretically possible for all episode days at the 80% NOx emission levels with varying IOLE emission reductions, albeit fairly large emission reductions in some cases. For the 85% NOx emission reduction level, compensation potential again varies by day and compensating NOx emission reductions with IOLE emission reductions would be possible at a number of industrial olefin emission levels. In general, based on the results of the sensitivity simulations, increased NOx emissions results in broad regions of ozone concentration increases while reductions in industrial olefin emissions produce more localized ozone reductions.

Given the limitations inherent with the sensitivity modeling performed for this study, it would be advantageous to consider various refinements to the sensitivity simulations. Because the alternative emission scenarios have been developed based on model-ready data, the identification and adjustments for industrial sources were based on the assumption that all point source emission are due to industrial sources. While this may be true for the majority of sources, a more refined analysis based on raw inventory data is likely to provide a more realistic representation of the impacts due modeled ozone concentrations due to the various future year control strategies. In addition, the refinement of the olefin and VOC emission scenarios with respect to varying either pollutant independently or in combination with other industrial VOC emission components may provide additional insight to the results presented here.

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