Final Report

SENSITIVITY ANALYSES OF THE SEPTEMBER 8-11, 1993 OZONE EPISODE

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1. INTRODUCTION

The 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 purpose of this study is to apply new features of the CAMx model to the 8-11 September, 1993 ozone episode 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. Although the final SIP was based on the Strategy I8 emission inventory, Strategy I8a is used here as it includes a minor correction to the Strategy I8 inventory.

OBJECTIVES

The overall objectives of this study are as follows:

1. Apply new features of the CAMx model to the 8-11 September, 1993 ozone episode and evaluate model performance. The latest version of CAMx, version 3.01, is applied and compared with the modeling results using CAMx version 2.03, which was used in the 2000 SIP revision. Both the flexi-nesting and chlorine chemistry features of CAMx version 3.01 are then applied and model performance evaluated using the statistical and graphical analyses recommended by EPA Guidance.

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. Adjustments to the VOC emission inventory are made based on the TexAQS Special Inventory and upset/maintenance reports compiled from EPA Region 12 databases in order to characterize the types of non-routine emissions that are known to occur in the industrial areas.

3. Determine the level of VOC emission reductions necessary to achieve the same peak ozone levels as Strategy I8a and the necessary VOC emission reductions required to compensate for the remaining NOx emission reductions.

This report documents and discusses the CAMx modeling performed to investigate the second and third objectives listed.

2. TECHNICAL APPROACH

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 in order 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 8 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.

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; ENVIRON and MRC, 2001) and CAMx model performance evaluations using these alternative meteorological fields have been performed and documented (Tesche and McNally, 2001).

The 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. The anthropogenic point, area, and nonroad mobile emission inventories were prepared using SMOKE (http://envpro.ncsc.org/products/smoke/), while the on-road mobile source emissions were processed using Fast-EPS. Biogenic emission inventories were prepared using the GLOBEIS2 model (http://www.globeis.com). The chlorine emission inventory used for this study was prepared by the University of Texas at Austin (UT) and is described in detail elsewhere (Tanaka and Allen, 2001). The chlorine emission estimates provided by UT were processed using the emissions preprocessor system version 2 (EPS2) and formatted for CAMx. Boundary and initial conditions were developed by the TNRCC using methods developed in Yocke et al.,

1996. The TNRCC provided the CAMx input files for the September 1993 episodes while the original CAMx simulation control files were provided by MCNC.

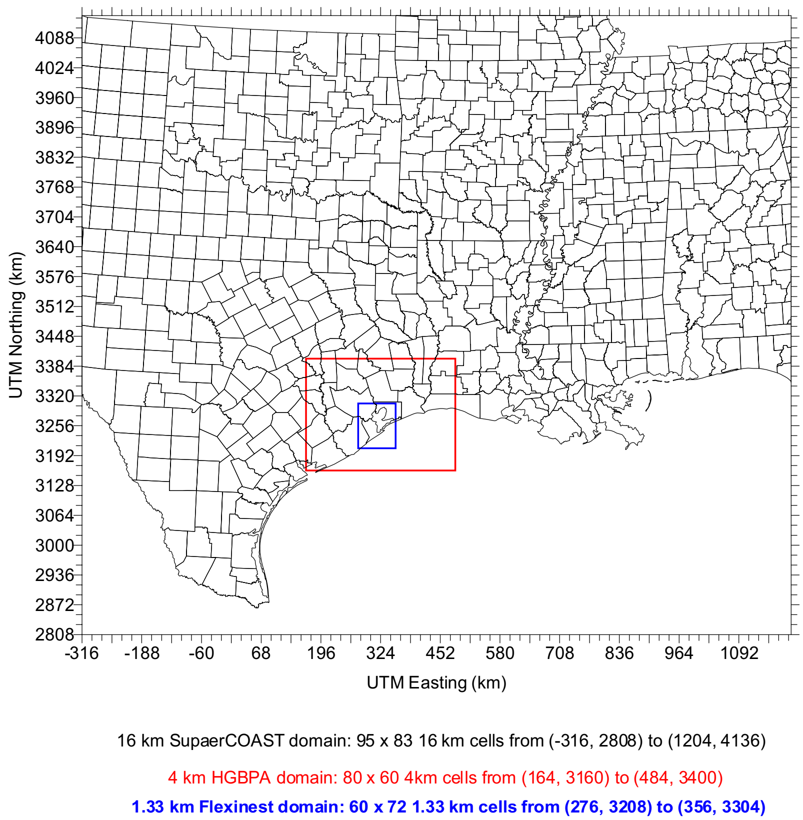


Figure 2-1. Map of the SuperCOAST domain showing the location of the 4-km HGBPA and 1.33 km Flexi-nest domains.

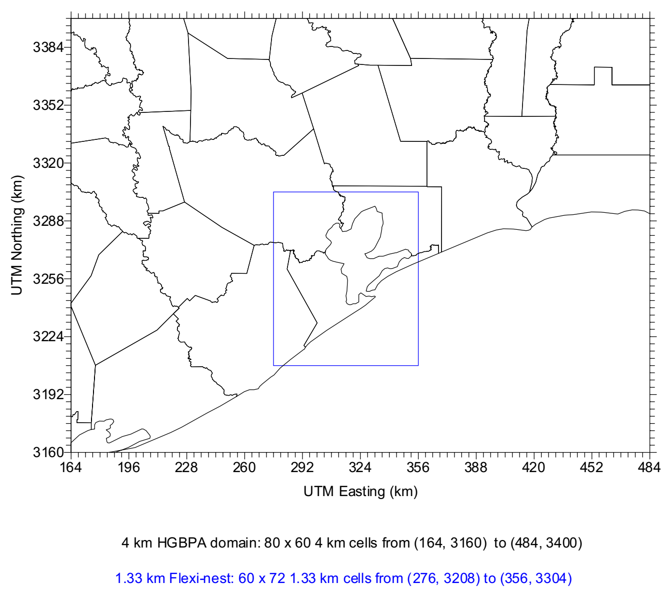


Figure 2-2. Map of the 4-km HGBPA domain showing the location of the 1.33-km Flexi-nest grid.

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. ENVIRON subsequently performed a comparison of the 2007 future year scenario using CAMx versions 1.13 and 2.03 (ENVIRON, 2000). The comparison study resulting in small differences in the modeled ozone between CAMx v1.13 and v2.03 with differences in the daily maximum ozone on the order of 1 ppb. Subsequently, the TNRCC revised the SIP modeling demonstrations using CAMx version 2.03 and developed the December 2000 SIP revision. Under Task 2 of the present study a number of sensitivity simulations were performed to investigate the impact of model versions, domain configuration and chlorine chemistry on model performance for the September 1993 episode. The simulations evaluated the model performance for CAMx versions 2.03 and 3.01 as well as the effect of chlorine chemistry. In addition, the inclusion of a high-resolution 1.33-km nested grid encompassing the Houston Ship Channel and Galveston Bay was investigated. The impact on model performance of alternative advection schemes was also considered. The results of these sensitivity simulations are documented in ENVIRON (2002). Briefly, the following conclusions can be drawn from the results of the analyses performed under Task 2:

- All model configurations evaluated (CAMx versions 2.03 and 3.01, CAMx version 3.01 with chlorine chemistry, CAMx version 3.01 with a 1.33-km nested grid and CAMx version 3.01 with the PPM advection scheme) result in acceptable model performance with respect to EPA guidance. Statistical measures of peak accuracy, normalized bias and normalized gross error all meet the goals set forth by the EPA for SIP modeling demonstrations.

- Based on the differences in modeled concentrations of daily maximum 1-hour ozone in the Houston urban area and more generally within the SuperCOAST modeling domain, the application of version 3.01 of CAMx instead of version 2.03 would not significantly change the response to emissions scenarios used by the TNRCC for control strategy evaluation.

- Given the uncertainties and biases believed to exist in key model inputs, such as the SAIMM meteorology and the industrial emissions, we conclude that model performance is similar for all of the model configurations evaluated here and that the model configuration for use in further studies should be selected based on the best science.

The results of the model evaluations performed under Task 2 led to the recommendation to use version 3.01 of the CAMx model for further emission sensitivity simulations. The model configuration should make use of the updated chlorine chemistry and include 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 flexi-nest, the PPM advection scheme and no Plume-in-Grid treatment of elevated point source emissions.

In order to further quantify the impact on modeled ozone concentrations due to the various model versions and domain configurations, the rate of ozone production within the HGBPA 4-km domain was evaluated. Table 2-1 displays the results of the analysis that 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, defined as the maximum difference from hour to hour of the average ozone concentration anywhere within the 4-km HGBPA modeling domain, for the 1993 base case simulations was evaluated for Version 2.03 and Version 3.01 of the CAMx model as well as for the simulations using version 3.01 with chlorine chemistry, flexi-nesting and using the Piece-wise Parabolic Method (PPM) advection scheme. The rate of ozone production is seen to increase as one goes from version 2.03 to version 3.01 as well as with the implementation of chlorine chemistry and increased resolution through the use of the flexi-nesting capabilities of the model.

Table 2-1. Comparison of peak ozone production rate.

	Peak Ozone Production Rate (ppb/hr)			
Model Version	**Sept. 8, 1993**	**Sept. 9, 1993**	**Sept.10, 1993**	**Sept. 11, 1993**
CAMx v2.03	34.8	32.5	46.3	37.9
CAMx v3.01	37.8	33.7	47.3	41.6
CAMx v3.01 w/Cl & Flexi-nest (PPM Advection scheme)	52.4	60.5	62.0	60.3

The effect of chlorine chemistry on the peak ozone production rate is illustrated Table 2-2. In this case the calculation of ozone production rates was confined to a small regions centered on Texas City where the largest sources of chlorine emission are present. The impacts due to chlorine chemistry are not large likely because of rapid ozone production from other emission sources at other times of the day.

Table 2-2. Effect of chlorine chemistry on peak ozone production rate.

	Peak Ozone Production Rate (ppb/hr)			
Model Version	**Sept. 8, 1993**	**Sept. 9, 1993**	**Sept.10, 1993**	**Sept. 11, 1993**
CAMx v3.01	37.8	33.7	47.3	41.6
CAMx v3.01 w/Cl	37.8	34.9	47.2	41.3

In order to document the input data that were used, as well as the CAMx version 3.01 model configuration, the CAMx control files for the first day of the September 1993 future year episode and for the first day with the implementation of the flexi-nest are shown in Figures 2-3 and 2-4, respectively.

```
Version             |VERSION3
Message string      |CAMx SuperCOAST base : one HG/BPA 4x4km subgrid, 930906 V3.01 (ENVIRON 12/27/01)
Root output name    |../../output/base/camx3.930906.base
Start time/date     |1993 09 06    0.
End time/date       |1993 09 06 2400.
DT:max,in,emis,out  |0.5 1. 1. 1.
nx,ny,nz            |95  83  8
Coordinate ID       |UTM
xorg,yorg,dx,dy,uzn |-316. 2808.  16.  16.  15
time zone           |6
PiG parameters      |2000. 12.
Avg output species  |1
                    |O3
Num fine nest       |1
net grid params     |31 50 23 37  8  4
SMOLAR or BOTT?     |PPM
Solver              |CMC
Restart             |false
Chemistry           |true
Dry dep             |true
Wet dep             |false
PiG submodel        |false
Staggered winds     |false
Treat area emiss    |true
Treat point emiss   |true
1-day emiss inputs  |true
3-D average file    |false
Source Apportion    |false
Chemparam           |/disk22/tnrcc/camx/input/common/CAMx3.chemparm.3.cl.noBUTA.sens
Photolysis rates    |/disk22/tnrcc/camx/input/common/camx_photorate.930906-
930911.isop.tcas_16km+hgbpa_04km.better
Landuse             |/disk22/tnrcc/camx/input/common/uamv_landuse.super_16km
Height/pressure     |/disk22/tnrcc/camx/input/met/uamv_zp.930906.tcas_16km
Wind                |/disk22/tnrcc/camx/input/met/uamv_wind.930906.super_16km.CAMx2
Temperature         |/disk22/tnrcc/camx/input/met/uamv_temp.930906.super_16km.CAMx2
Water vapor         |/disk22/tnrcc/camx/input/met/uamv_h2o.930906.super_16km
Cloud cover         |
Rainfall            |
Vertical diffsvty   |/disk22/tnrcc/camx/input/met/uamv_kv.930906.super_16km
Initial conditions  |/disk22/tnrcc/camx/input/common/camx2.930905.93basAj.ic.bin
Boundary conditions|/disk22/tnrcc/camx/input/bc-ic-tc/93basAj/uamv_bc.930906
Top concentration   |/disk22/tnrcc/camx/input/bc-ic-tc/93basAj/uamv_tc.clean
Albedo/haze/ozone   |/disk22/tnrcc/camx/input/common/uamv_aho.930906-930911.tcas_16km+hgbpa_04km
Point emiss
|../../input/emiss/elpts.93base.base/egts.allpts.19930906.93base.base.super.cl.a0.bin
Area emiss          |/disk22/tnrcc/camx/input/emiss/aak93/low_ei.super16km.19930906.93babb.bin
Landuse          #1 |/disk22/tnrcc/camx/input/common/uamv_landuse.hgbpa_04km
Height/pressure #1 |/disk22/tnrcc/camx/input/met/uamv_zp.930906.hgbpa_04km
Wind             #1 |/disk22/tnrcc/camx/input/met/uamv_wind.930906.hgbpa_04km.CAMx2
Temperature      #1 |/disk22/tnrcc/camx/input/met/uamv_temp.930906.hgbpa_04km.CAMx2
Vertical diff    #1 |/disk22/tnrcc/camx/input/met/uamv_kv.930906.hgbpa_04km
Area emiss       #1 |../../input/emiss/93base.base/low_ei.4km.19930906.93base.base.bin
Coarse grid restart|
Fine grid restart  |
PiG restart         |
```

Figure 2-3. CAMx (version 3.01) control file (CAMx.in) for the September 6, 1993 base year episode day.

```
Version             |VERSION3
Message string      |CAMx SuperCOAST base : one 4x4km subgrid + 1.33km Flex, 930908 V3.01 (ENVIRON
12/27/01)
Root output name    |../../output/base/camx3.930908.base
Start time/date     |1993 09 08    0.
End time/date       |1993 09 08 2400.
DT:max,in,emis,out  |0.5 1. 1. 1.
nx,ny,nz            |95  83  8
Coordinate ID       |UTM
xorg,yorg,dx,dy,uzn|-316. 2808.  16.  16.  15
time zone           |6
PiG parameters      |2000. 12.
Avg output species  |1
                    |O3
Num fine nest       |2
nest grid params    |31 50 23 37  8  4
nest grid params    |38 42 26 31  8 12
SMOLAR or BOTT?     |PPM
Solver              |CMC
Restart             |true
Chemistry           |true
Dry dep             |true
Wet dep             |false
PiG submodel        |false
Staggered winds     |false
Treat area emiss    |true
Treat point emiss   |true
1-day emiss inputs  |true
3-D average file    |false
Source Apportion    |false
Chemparam           |/disk22/tnrcc/camx/input/common/CAMx3.chemparm.3.cl.noBUTA.sens
Photolysis rates    |/disk22/tnrcc/camx/input/common/camx_photorate.930906-
930911.isop.tcas_16km+hgbpa_04km.better
Landuse             |/disk22/tnrcc/camx/input/common/uamv_landuse.super_16km
Height/pressure     |/disk22/tnrcc/camx/input/met/uamv_zp.930908.tcas_16km
Wind                |/disk22/tnrcc/camx/input/met/uamv_wind.930908.super_16km.CAMx2
Temperature         |/disk22/tnrcc/camx/input/met/uamv_temp.930908.super_16km.CAMx2
Water vapor         |/disk22/tnrcc/camx/input/met/uamv_h2o.930908.super_16km
Cloud cover         |
Rainfall            |
Vertical diffsvty   |/disk22/tnrcc/camx/input/met/uamv_kv.930908.super_16km
Initial conditions  |
Boundary conditions|/disk22/tnrcc/camx/input/bc-ic-tc/93basAj/uamv_bc.930908
Top concentration   |/disk22/tnrcc/camx/input/bc-ic-tc/93basAj/uamv_tc.clean
Albedo/haze/ozone   |/disk22/tnrcc/camx/input/common/uamv_aho.930906-930911.tcas_16km+hgbpa_04km
Point emiss
|../../input/emiss/elpts.93base.base/egts.allpts.19930908.93base.base.super.cl.a0.bin
Area emiss          |/disk22/tnrcc/camx/input/emiss/aak93/low_ei.super16km.19930908.93babb.bin
Landuse          #1 |/disk22/tnrcc/camx/input/common/uamv_landuse.hgbpa_04km
Landuse          #2 |
Height/pressure #1 |/disk22/tnrcc/camx/input/met/uamv_zp.930908.hgbpa_04km
Height/pressure #2 |
Wind             #1 |/disk22/tnrcc/camx/input/met/uamv_wind.930908.hgbpa_04km.CAMx2
Wind             #2 |
Temperature      #1 |/disk22/tnrcc/camx/input/met/uamv_temp.930908.hgbpa_04km.CAMx2
Temperature      #2 |
Vertical diff    #1 |/disk22/tnrcc/camx/input/met/uamv_kv.930908.hgbpa_04km
Vertical diff    #2 |
Area emiss       #1 |../../input/emiss/93base.base/low_ei.4km.19930908.93base.base.bin
Area emiss       #2 |
Coarse grid restart|../../output/base/camx3.930907.base.inst.2
Fine grid restart   |../../output/base/camx3.930907.base.finst.2
PiG restart         |
```

Figure 2-4. CAMx (version 3.01) control file (CAMx.in) for September 8, 1993 including the specification of the 1.33-km Flexi-nested grid.

3. EMISSION SCENARIOS

The overall 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. For the future year Strategy I8a scenario, an investigation of greater industrial VOC emission reductions required to compensate for lesser industrial NOx emission reductions contained in the final 2000 SIP was also conducted. The alternative emission scenarios will examine the effect of increased emissions of volatile organic compound from industrial sources (industrial VOC, or IVOC), both continuously and episodically. 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). In addition, from an analysis of the TexAQS Special Inventory and upset/maintenance reports, a number of episodic upset emission scenarios were developed and examined in order to evaluate the effects of non-routine emissions occurring within the industrial areas around the Houston Ship Channel and Galveston Bay.

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 the current study makes 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 are accomplished using the EPS2 utility processors to apply appropriate adjustment factors to the elevated and low level NOx and/or VOC emissions.

Two series of future year emission scenario simulations were conducted. The first series considered preliminary simulations, applied emission adjustments to all industrial sources within the entire 4-km HGBPA modeling grid. These scenarios did not distinguish between existing and new sources for the purpose of adjusting NOx emission levels from the 90% reductions in the SIP, nor were ship emissions excluded from emission changes (the TNRCC treated shipping emissions as elevated point sources). These runs were performed to quickly evaluate the various emission scenarios prior to the development of the necessary data and processing procedures to correctly account for sources not subject to controls, including new sources and ship emissions, and to confine emission adjustments to the 8-county Houston-Galveston area. The final series of future year emission scenarios were performed with these issues taken into consideration.

This section of the report documents the development of 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 and episodic 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 3-1 presents a summary of existing emissions in the September 1993 base year emission inventory.

Table 3-1. 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 in total VOC as well as industrial light olefins (IOLE, represented by modeled species ETH and OLE), both separately and in combination with each other. In consultation with TNRCC staff, the sensitivity scenarios for continuous IVOC emission increases identified for evaluation are presented in Table 3-2. These scenarios were conducted to determine a more realistic level of VOC emissions consistent with findings of the TexAQS. Each of these scenarios were simulated using the CAMx air quality model and the resulting model performance was evaluated with respect to EPA guidance on acceptable model performance. The simulation which resulted in model performance on the edge of the acceptable limits was chosen as representative of actual atmospheric pollutant levels for the 1993 base year.

Table 3-2. Summary of 1993 Base Year Alternative Industrial VOC Emission Scenarios

Scenario Name	IVOC Increase (%)[1]	IOLE Increase (%)
200ole.200voc	100	100
200ole.250voc	150	100
200ole.300voc	200	100
300ole.200voc	100	200
300ole.250voc	150	200
300ole.300voc	200	200

[1] Emission adjustments are multiplicative, i.e., IVOC increases are applied in addition to IOLE increases.

The above scenarios were developed through application of the appropriate adjustment factors using the emission processing utilities, MRGUAM and PTSCOR for low level and elevated point sources, respectively.

A number of experimental episodic emission scenarios were also examined. Based on consultations with the TNRCC project manager, a VOC upset condition occurring at the Baytown Olefins Plant was selected to evaluate the effects of episodic VOC emission increases on model performance. Specifically, a release of ethylene at a rate of 5000lb/hr between 4 am and 8 am September 8, 1993. Also considered was a release of propylene at the same rate and location. The release point was chosen as 303.637 km Easting, 3292.915 km Northing, UTM Zone 15, which corresponds to a location near Baytown at the mouth of the Houston Ship

Channel. The specific location was chosen based on an examination of model wind back trajectories ending at Smith Point and Seabrook at around mid-day September 8, 1993. In order to ensure that the upset emissions were released within the lowest model layer, the emissions were added to the low-level component emissions data file. In addition, minor adjustments with respect to the time of release and upset duration were also considered. Table 3-3 summarizes the upset scenarios simulated.

Table 3-3. Summary of Upset Emission Scenarios.

Scenario Name	Emission release (magnitude and species)	Release duration (start and end time, Sept. 8, 1993)
UPSET1	5000 lb/hr Ethylene (ETH)	4 am – 8 am
UPSET1A	5000 lb/hr Ethylene (ETH)	5 am – 10 am
UPSET1B	5000 lb/hr Ethylene (ETH)	5 am – 11 am
UPSET1C	5000 lb/hr Propylene (OLE+PAR)	5 am – 11 am

Another emission sensitivity simulation performed for the 1993 base year was derived from an analysis of measured Olefin/NOx ratios presented by Sonoma Technology, Inc. presented at the 2002 Annual Meeting of the American Meteorological Society (STI, 2002). The results of the STI study, developed through analyses of continuous measurements of concentrations of ozone and ozone precursors obtained from aircraft flights around several major industrial facilities within the Houston urban area, indicated a relation between measured levels of alkenes and NOx from industrial sources. The study concluded that preliminary observed ratios of alkenes to NOx were on the order of 0.5-2:1 (ppb olefin per ppb NOx). Thus, this formed the basis of the emission sensitivity simulation referred to in the current study as SENS2. The specific geographic area in which the emission adjustments were applied was based on the example flight path displayed in the STI presentation, which circled several industrial facilities located near the Houston Ship Channel including plants in Baytown, Channelview, Deer Park, Clear Lake and Mont Belvieu. Due to the need to develop the emission scenarios based on model ready emissions data files, the region was approximated by selecting a small subregion within the HGBPA 4-km domain, and applying adjustments to the appropriate modeled pollutants within the elevated point source data file. In particular, model species ETH, OLE and PAR were replaced, on a molar basis, with 0.5NOx emissions for each point source within the selected subregion. This is equivalent to an olefin to NOx ratio of 1, with the olefins split between 50% ethene and 50% propene. Figure 3-1 displays the location of the subregion to which these adjustments were made. These changes result in the following emission increases in tons per day (tpd) for PAR, ETH, and OLE, respectively: 230 tpd; 673 tpd; and 672 tpd

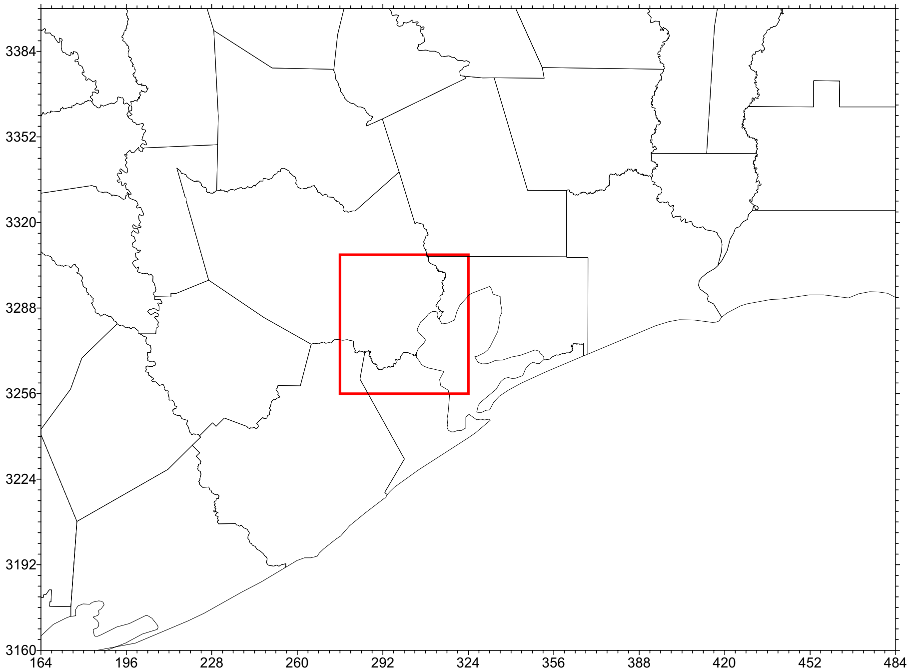


Figure 3-1. Location of subregion for emission adjustments under emission scenario SENS2. Note that only elevated point sources are adjusted within this region and only for the SENS2 scenarios**.**

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 VOC emission levels. The CAMx model was then applied to determine the extent to which the modeled ozone concentrations could be reduced to the Strategy I8a levels through reduction of industrial VOC 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 3-4 presents to VOC and NOx emission totals within and outside the HGBPA 4-km modeling domain. Table 3-5 provides a summary of the preliminary across-the-board industrial NOx and VOC emission reduction scenarios considered. Note that the "80n100v" scenario represents the 2007 future year emission levels without the SIP adopted NOx reductions. This simulation, therefore, represents the starting point for the investigation of potential VOC reduction scenarios to compensate for the proposed NOx reductions. Of note is the "80n00v" scenario, which corresponds to the maximum potential industrial VOC emission reductions. An investigation was also undertaken to determine the potential of compensating for industrial NOx emission reductions with reductions in industrial olefins alone. The emission scenarios developed for this investigation are listed in Table 3-6.

Table 3-4. NOx and VOC Strategy I8a Emission Summaries within and outside the 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 3-5. Summary of Preliminary 2007 Strategy I8a Emission Scenarios

Scenario Name	INOx Increase (%)	IVOC Increase (%)	IOLE Increase (%)
00n00v	-100	-100	0
80n00v	100	-100	0
80n1000v	100	900	0
80n100v	100	0	0
80n300v	100	200	0
80n600v	100	500	0
80n10v	100	-90	0
80n20v	100	-80	0
80n30v	100	-70	0
80n40v	100	-60	0
80n50v	100	-50	0
80n60v	100	-40	0
80n70v	100	-30	0
80n80v	100	-20	0
85n00v	50	-100	0
85n50v	50	-50	0
90n300v	0	200	0
90n600v	0	500	0
90n1000v	0	900	0
IOLE2	0	0	100
IOLE5	0	0	400
IOLEx290n300v	0	200	100
IOLEx290n600v	0	500	100
IOLEx290n1000v	0	900	100
IOLEx590n300v	0	200	400
IOLEx590n600v	0	500	400
IOLEx590n1000v	0	900	400

Table 3-6. Summary of Additional Preliminary 2007 Strategy I8a Emission Scenarios.

Scenario Name	INOx Increase (%)	IVOC Increase (%)	IOLE Increase (%)
0.0ole.80nox	100	0	-100
0.2ole.80nox	100	0	-80
0.5ole.80nox	100	0	-50
0.7ole.80nox	100	0	-30
1.0ole.80nox	100	0	0
1.2ole.80nox	100	0	20
1.5ole.80nox	100	0	50
2.5ole.80nox	100	0	150
3.5ole.80nox	100	0	250
0.0ole.85nox	50	0	-100
0.2ole.85nox	50	0	-80
0.5ole.85nox	50	0	-50
0.7ole.85nox	50	0	-30
1.0ole.85nox	50	0	0
1.2ole.85nox	50	0	20
1.5ole.85nox	50	0	50
2.5ole.85nox	50	0	150
3.5ole.85nox	50	0	250

As with the 1993 base year simulations, a number of episodic emission reduction scenarios were considered for the 2007 Strategy I8a simulations. These were defined to be the same as in the base year, applied to the 2007 projected emission levels, and for the UPSET scenarios are summarized in Table 3-3. Application of the SENS2 emission scenario resulted in the following emission increases in tons per day (tpd) for PAR, ETH, and OLE, respectively: 19 tpd; 69 tpd; and 69 tpd

Each of the above alternative emission scenarios were simulated using Version 3.01 of the CAMx air quality model, configured as discussed above in Section 2.

Identification of the "Shipping Sources"

The refinement of the future year alternative emission scenarios involved the identification of shipping emissions, accounting for new sources not subject to controls and the restriction of the emission adjustments to the 8-county Houston-Galveston area.

Ships were located by matching "stack parameters" in the 2007 shipping "AFS" file to stack parameters in the model ready elevated point source file. This means matching sources based on location. Locations were considered a match when they agreed to within 10 meters. The 10-meter tolerance is necessary to account for the limits of representing these locations as 4-byte real binary numbers plus several conversions between binary and ASCII format.

Figure 3-2 shows the location of elevated sources identified as ships. They follow the ship channel and intra-coastal waterway, as expected.

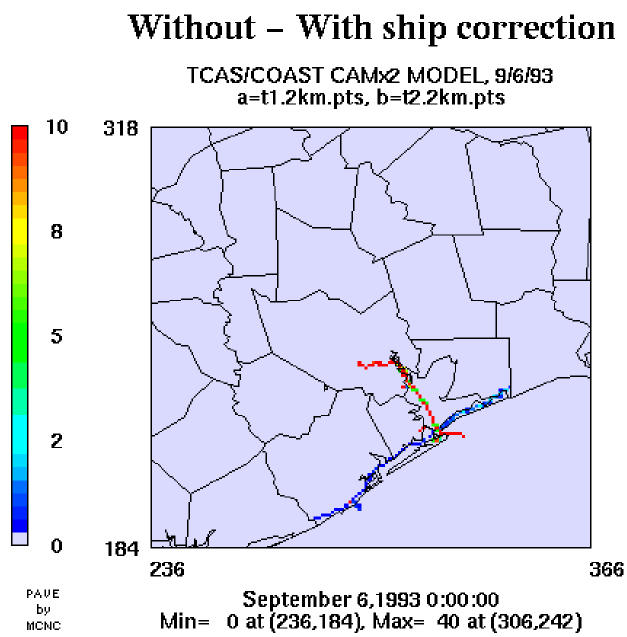


Figure 3-2. Location of shipping emission sources.

Scaling Emissions from "Industrial Sources"

Emissions from industrial sources were identified as follows:

- Elevated points within a 4 km resolution mask of the 8-county Houston-Galveston area that were not ships
- Low level points within a 4 km resolution mask of the 8-county Houston-Galveston area

The 4-km resolution mask of the 8-county Houston-Galveston area was provided by the TNRCC. Figure 3-3 below shows the location of elevated NOx point sources resolved to 2-km grid cells. The graphics also show the ratio of elevated point NOx emissions when the "INOx" sources are doubled.

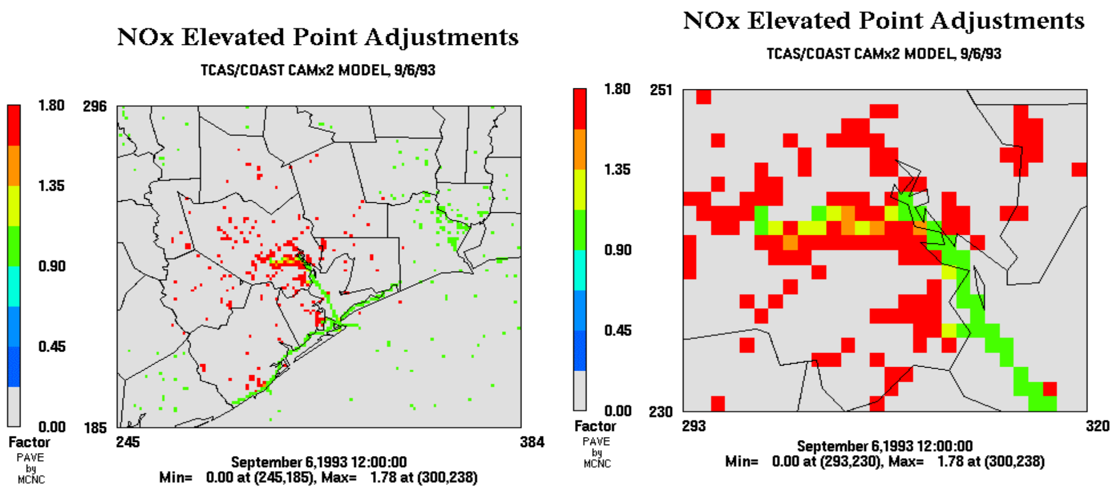


Figure 3-3. Industrial NOx elevated point source locations.

Emissions from the "INOx" sources were "doubled" and appear in red in Figure 3-3. Doubling amounts to multiplying by a factor of 1.78 to account for new sources not subject to control. The factor of 1.78 was obtained through consideration of the industrial NOx emission levels in the i8 Strategy within the 8-county area and the NOx emission levels from new sources. The i8 Strategy contained 103 tons of industrial NOx in the 8-county area, of which 23 tons were from new sources. Therefore, to multiply the controlled sources by 2 we multiply all industrial sources by the following: [2 x (103-23) + 23]/103 = 1.78. Ships and sources outside the 8-county mask were not doubled and appear in green. In the detail of the ship channel area, some 2-km grid cells contain both ships and INOx sources and appear yellow/orange.

Figure 3-4 shows the location of low level "INOx" point sources resolved to a 2-km grid. Sources are confined to the 8-county Houston-Galveston area.

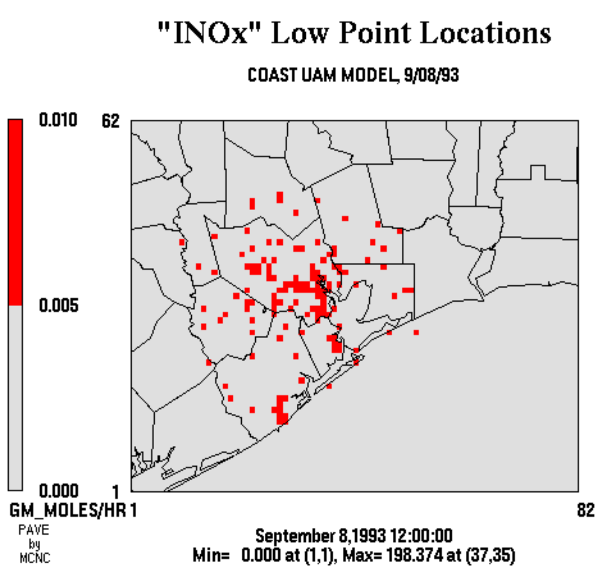


Figure 3-4. Low level industrial NOx point source locations.

The increase in NOx emissions between the i8 base inventory and the inventory with "doubled" industrial NOx emissions was 71 tons. This means that the base inventory had (71/0.78) = 91 tons of INOx. The shipping emissions amount to 39 tons of NOx.

Figure 3-5 displays the locations of elevated and low level industrial VOC (IVOC) sources. The sources are confined to the area of the 8-county mask, and do not include the shipping lanes. The amount of industrial VOC emissions in the inventory with doubled VOC and doubled olefins (i.e., ETH and OLE) was 336 tons, of which 104 tons were elevated and 232 tons low level.

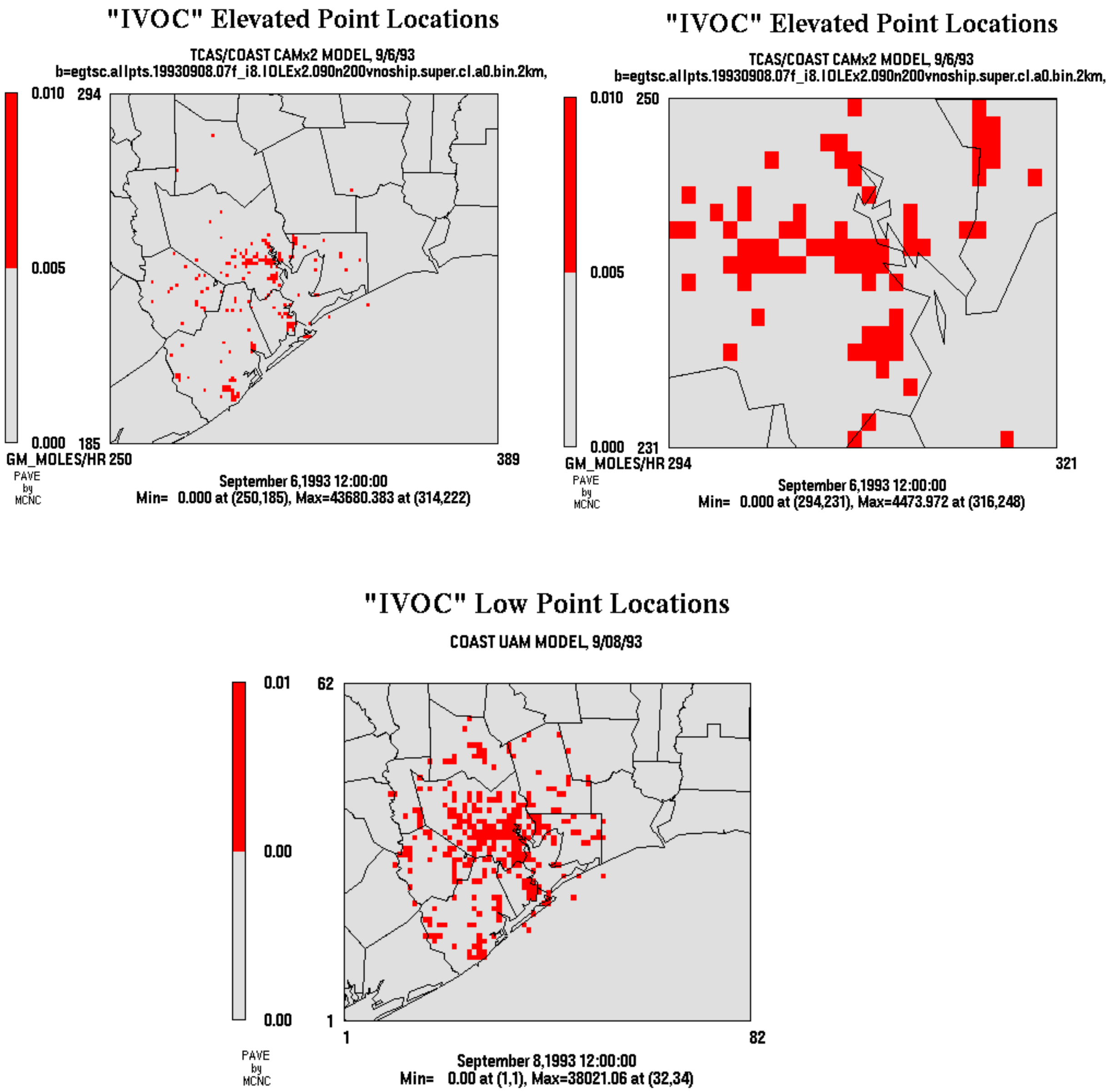


Figure 3-5. Industrial VOC point source locations

Based on model performance results of the 1993 base year VOC emission adjustment scenarios, the 2 x OLE/2 x VOC (200ole.200voc) simulation was selected as an acceptable alternative VOC emission level, consistent with findings of the TexAQS. The Strategy I8a inventory was adjusted to reflect the increased industrial VOC emission levels within the 8-county region. The resulting scenario was then simulated with CAMx to provide a reference for subsequent emission reduction scenarios. Two series of simulations were then undertaken; one with the industrial NOx emissions at 80% reduction levels from the base year and one with the industrial NOx emissions at 85% reductions levels from the 1993 base levels. Air quality model simulation were performed with each of these NOx reduction scenarios for varying levels of industrial VOC reductions to determine the potential for compensating NOx reductions in the future year with VOC emission reductions. The specific future year emission scenarios investigated are summarized in Table 3-7.

Table 3-7. Summary of future year 2007 alternative VOC emission scenarios.

Scenario Name	INOx Increase (%)	IVOC Increase (%)	IOLE Increase (%)
i8 200ole.200voc	0	100	100
80nox.0voc	100	-100	100
80nox.50voc	100	-50	100
80nox.100voc	100	0	100
80nox.150voc	100	50	100
80nox.200voc	100	100	100
85nox.0voc	50	-100	100
85nox.50voc	50	-50	100
85nox.100voc	50	0	100
85nox.150voc	50	50	100
85nox.200voc	50	100	100

4. MODELING RESULTS AND MODEL PERFORMANCE EVALUATION

The results of the emission sensitivity scenarios for both the 1993 base year and 2007 future year Strategy I8a are presented and discussed in this section.

1993 BASE YEAR

Each of the emission scenarios listed in Table 3-2, as well as the 1993 Base Case scenario, were simulated using version 3.01 of the CAMx air quality model using the model domain and configuration described in Section 2. The modeling results are examined and evaluated with respect to the spatial distribution of simulated daily maximum 1-hour ozone concentrations, the impacts of each emission scenario on the daily maximum 1-hour ozone concentrations and model performance evaluation criteria as defined by EPA guidance.

Figure 4-1 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 4-1, which also shows the peak modeled ozone concentration within the 4-km HGBPA domain. These data were compiled based on results at 1.33km horizontal resolution while most of the displays of spatial distributions are based on 4-km resolution modeling results.

Based on an examination of the model performance, and in consultation with the TNRCC, the 200ole.200voc emission scenario was determined to represent an appropriate level of VOC emissions while still maintaining acceptable model performance. This alternative VOC emission scenario was therefore selected as the starting point for the future year emission reduction scenarios. The spatial distribution of daily maximum 1-hour ozone concentrations within the 4-km domain for the 200ole.200voc emission scenario simulation is displayed in Figure 4-2.

An examination of Figures 4-1 and 4-2 reveals the effect of doubling industrial VOC and olefins on the estimated daily maximum 1-hour ozone concentrations. While the spatial distributions are similar, the peak ozone levels are increased and the locations of the peaks are slightly shifted on some days. Increases in peak ozone concentrations from the base case range from approximately 11 ppb on September 10 to more than 54 ppb on September 11. The September 8th and 9th days experience peak ozone increases of 23 ppb and 28 ppb, respectively. Figure 4-3 displays the difference in daily maximum 1-hour ozone concentrations between the 200voc.200ole emission scenarios and the 1993 base case simulation.

The model performance statistics presented in Table 4-1 show that for the 200ole.200voc scenario, the modeling exhibited acceptable performance with respect to EPA Guidance for all days and all measures except for the unpaired peak accuracy. In the table, highlighted entries indicate unacceptable model performance with respect to EPA guidance. The modeling results exceed acceptable limits considerably for the peak accuracy on the September 10th and 11th episode days. While nominally unacceptable by EPA standards, the failure to meet this goal may be related more to the location of ambient monitors with respect to modeled concentrations than to the inability of the model to replicate observed concentration levels.

The selection of the 200ole.200voc scenario as representative of realistic pollutant levels in the atmosphere in and around the Houston-Galveston region was made based on these model performance statistics, in consultation with the TNRCC Project Manager. This alternative emission scenario is the basis, or starting point, for future year control scenarios.

The effects of enhanced VOC emission on the ozone production rate for each of the 1993 base year sensitivity simulations are presented in Table 4.2

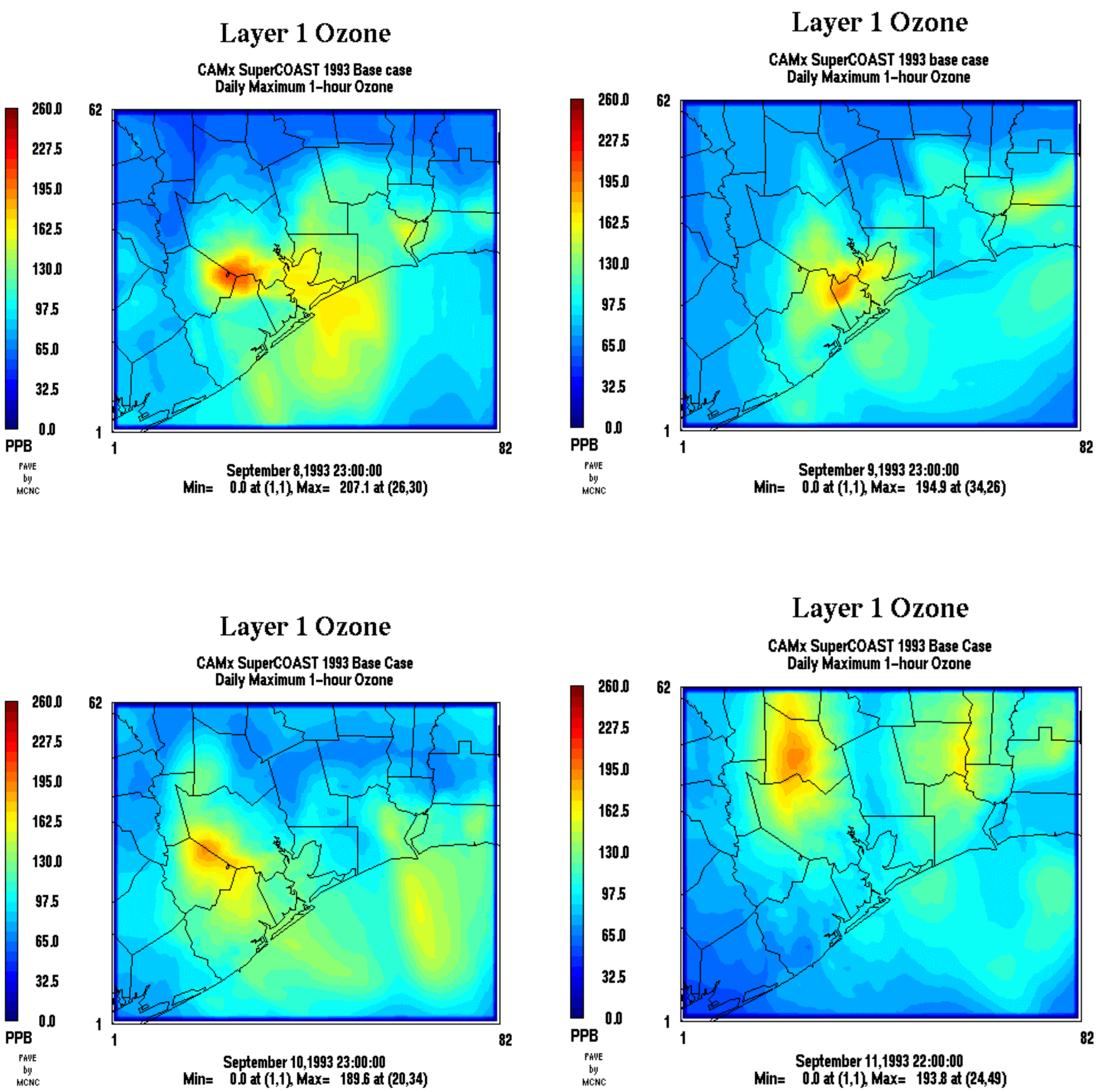


Figure 4-1. Daily maximum ozone concentrations for 1993 Base Case.

Table 4-1. 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 Base Case		207.1	198.0	189.6	193.8
200ole.200voc		232.4	230.6	202.3	251.7
200ole.250voc		240.4	241.4	212.4	265.0
200ole.300voc		247.4	251.7	225.8	274.3
300ole.200voc		242.8	246.2	217.9	268.5
300ole.250voc		256.2	258.6	233.9	280.0
300ole.300voc		269.4	267.2	245.1	287.9
SENS2		248.0	242.2	220.9	266.3
UPSET1C		207.1	-	-	-
Accuracy of Unpaired Peak (%)	< ±20%				
CAMx v3.01 Base Case		-3.2	1.5	17.1	2.5
200ole.200voc		8.6	18.3	24.9	33.2
200ole.250voc		12.4	23.8	31.1	40.2
200ole.300voc		15.6	29.1	39.4	45.1
300ole.200voc		13.5	26.3	34.5	42.1
300ole.250voc		19.7	32.6	44.4	48.2
300ole.300voc		25.9	37.0	51.3	52.3
SENS2		15.9	24.2	36.4	40.9
UPSET1C		-3.2	-	-	-
Mean Normalized Bias (%)	< ±15%				
CAMx v3.01 Base Case		7.1	5.3	-10.1	0.7
200ole.200voc		13.9	9.9	-2.7	11.4
200ole.250voc		14.9	10.9	-1.1	13.6
200ole.300voc		16.6	12.1	0.7	16.5
300ole.200voc		15.7	11.4	-0.2	14.5
300ole.250voc		17.9	13.1	2.3	18.4
300ole.300voc		21.7	15.4	5.5	24.3
SENS2		16.1	12.1	1.5	16.7
UPSET1C		-	-	-	-
Mean Normalized Gross Error (%)	< ±35%				
CAMx v3.01 Base Case		25.4	27.4	25.7	21.4
200ole.200voc		27.7	28.5	24.9	22.7
200ole.250voc		27.9	28.7	24.9	23.2
200ole.300voc		28.6	29.2	25.1	24.7
300ole.200voc		28.2	28.9	24.9	23.5
300ole.250voc		29.3	29.5	25.2	25.8
300ole.300voc		31.9	30.7	26.2	30.3
SENS2		28.4	29.1	24.5	24.7
UPSET1C		25.4	-	-	-

Table 4-2. Effect of VOC emission enhancements on peak ozone production rate (ppb/hr).

Scenario	8-Sep	9-Sep	10-Sep	11-Sep
200ole.200voc	62.84	61.75	64.96	78.56
200ole.250voc	65.45	66.86	66.25	83.34
200ole.300voc	67.68	77.10	70.63	86.10
300ole.200voc	66.89	74.69	67.04	87.22
300ole.250voc	70.47	87.21	79.24	90.05
300ole.300voc	80.11	99.43	96.79	98.85

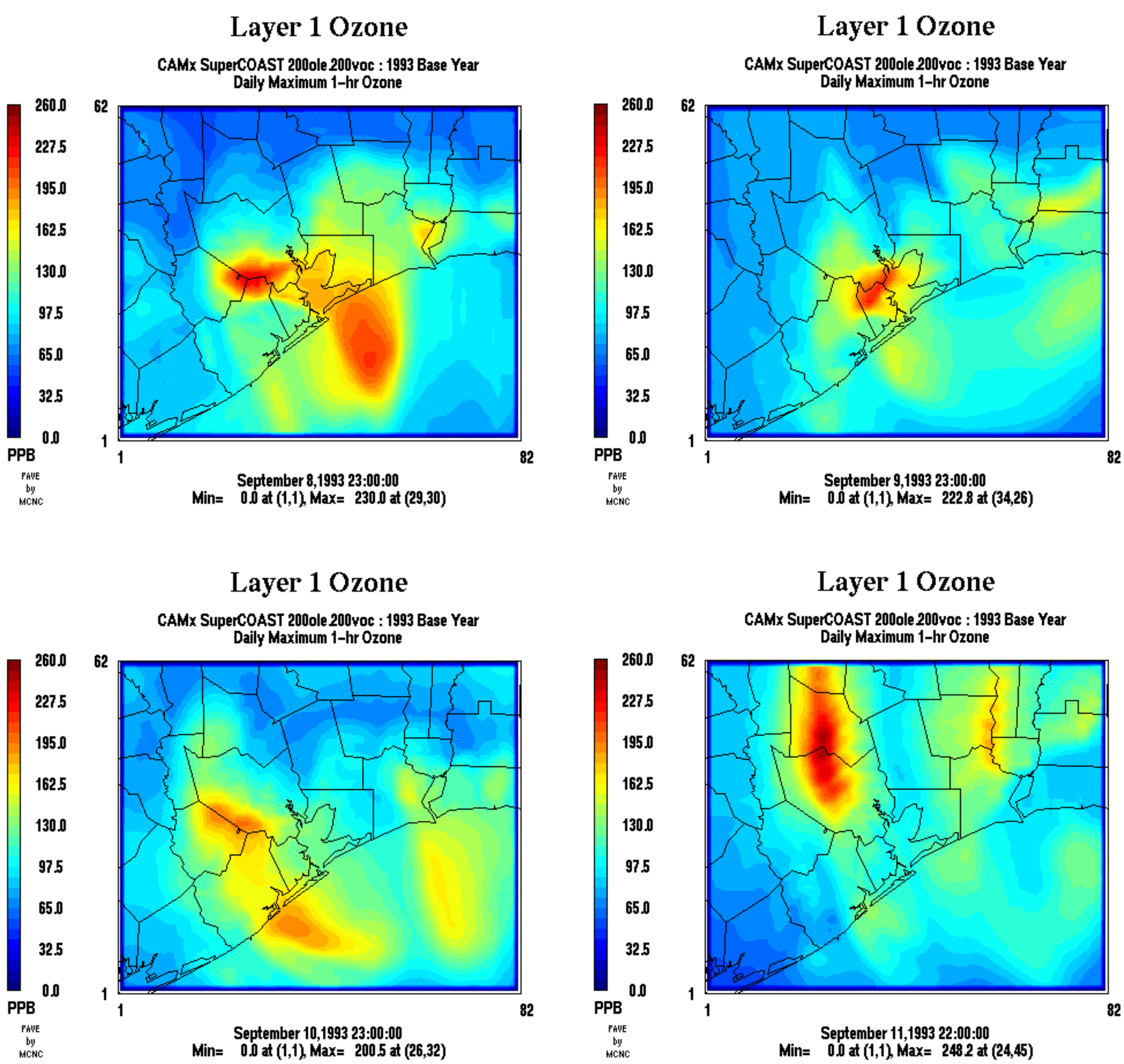


Figure 4-2. Daily maximum ozone concentrations for 1993 200ole.200voc scenario.

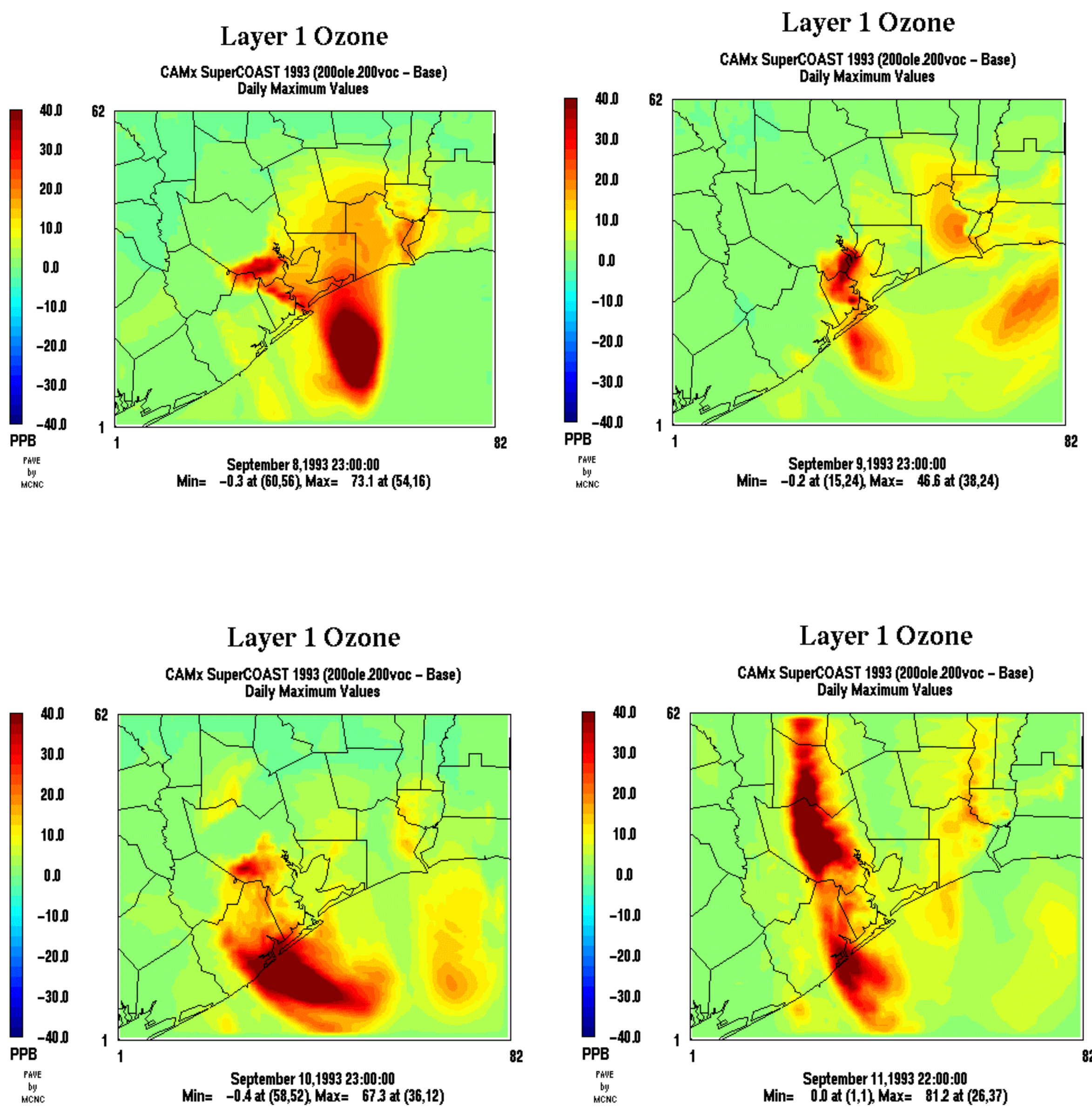


Figure 4-3. Difference in daily 1-hour maximum ozone for base year 1993. (200ole.200voc minus base case)

The effect of episodic VOC emission increases on the model performance is illustrated in Figure 4-4 and Figure 4-5. Figure 4-4 displays the impacts of the UPSET1C emission scenario. Displayed are the difference in simulated ozone concentrations between the UPSET1C scenario and the base case at 10:00 am on September 10, 1993. Also displayed is the difference in daily peak ozone concentrations. The impact on the daily peak ozone is seen to be a considerable increase (20 ppb) although highly localized around the ship channel in the area of the emission release. The effects at Seabrooke and Smith Point are illustrated in the difference isopleth at 10:00am, as well as in Figure 4-5, which displays time series for these two monitor locations. These results illustrate the capability of the CAMx model and associated databases to provide a reasonable representation of the impacts due to episodic, or non-routine, emission releases within the Houston-Galveston Bay area.

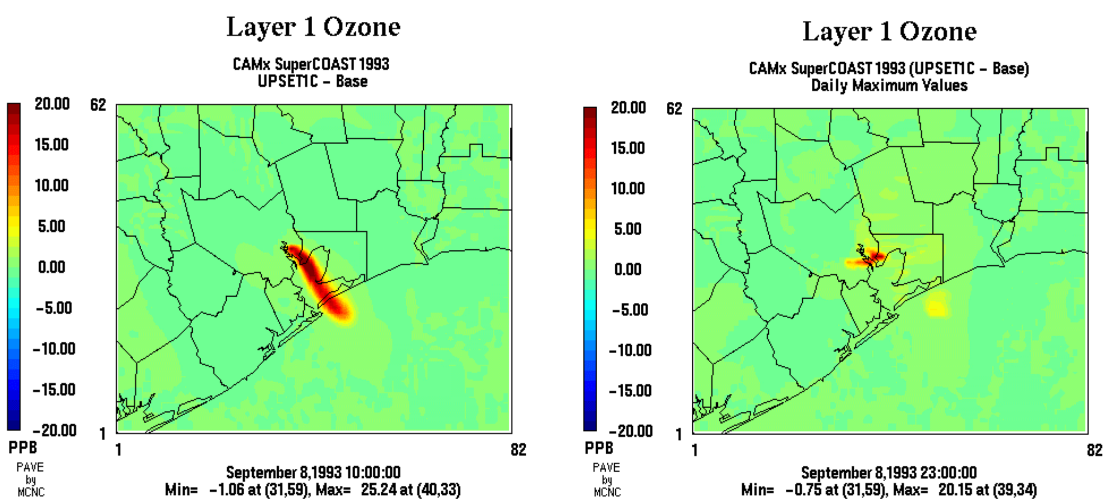


Figure 4-4. Ozone impacts under USET1C episodic emission scenario.

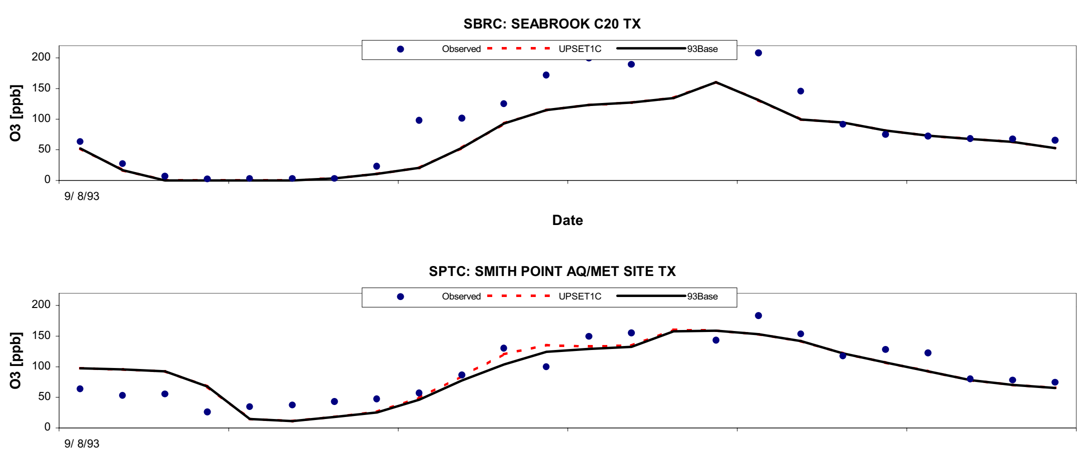


Figure 4-5. Times series plot for Seabrooke and Smith Point; Base case (solid line) and UPSET1C (dashed line).

The results of the SENS2 episodic emission scenario are presented in Figure 4-6. The difference in daily maximum 1-hour ozone concentrations between the SENS2 scenario and the 1993 base case are illustrated in terms of the spatial distribution of differences in peak ozone levels. Broad regions of relatively large ozone increases are realized generally downwind of the increased VOC emissions. Localized ozone increases are also seen. Increases in daily maximum ozone concentrations range from approximately 80 ppb to as much as 113 ppb, depending on the episode day. This sensitivity indicates the potential impact if equal amounts of olefins (ethene/propene) are co-released with the elevated NOx emissions.

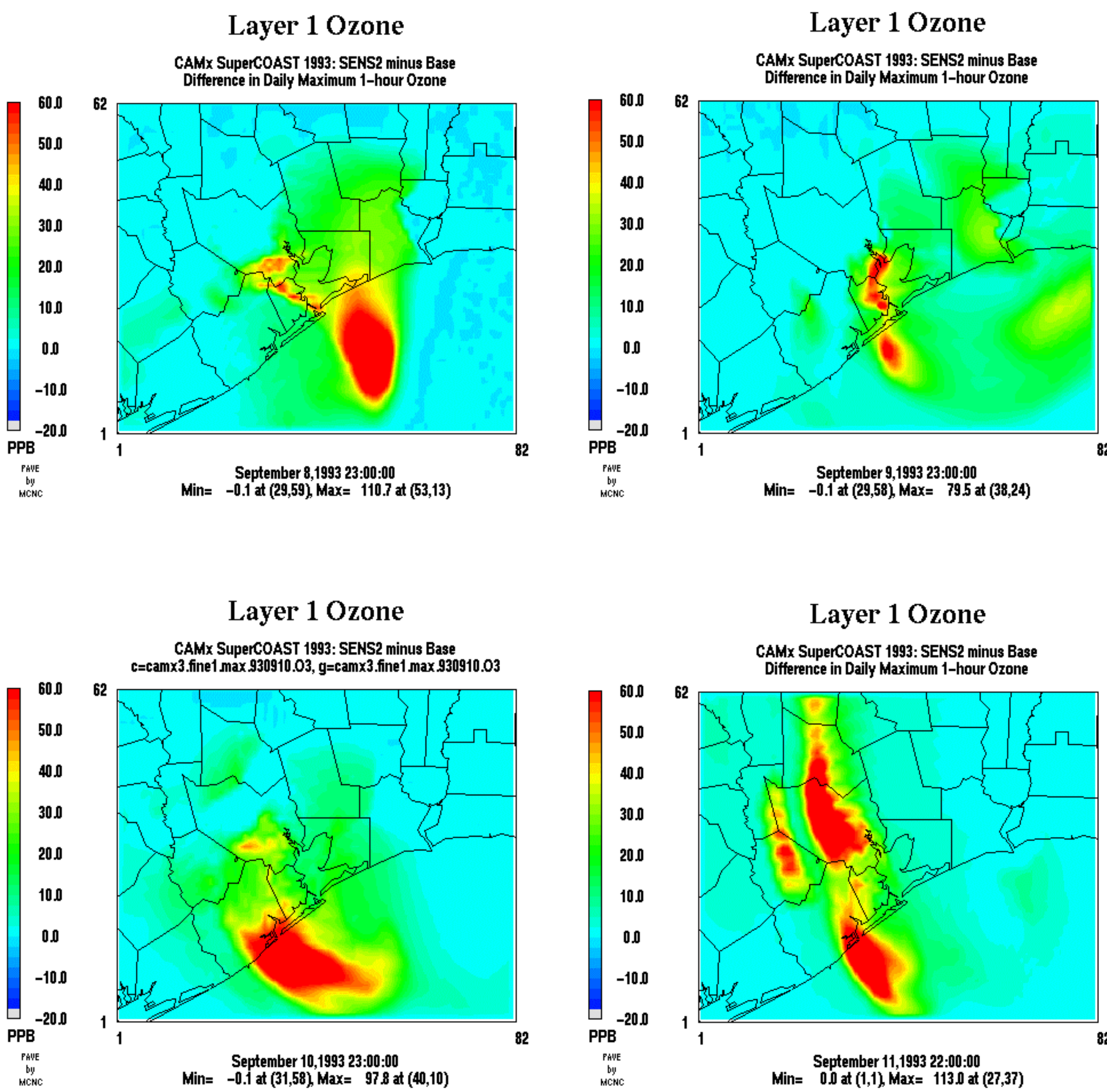


Figure 4-6. Impacts on daily maximum 1-hour ozone due to the SENS2 episodic emission scenario (elevated olefin emissions equal to elevated NOx).

2007 FUTURE YEAR SCENARIOS

Each of the emission scenarios developed for future year 2007 were simulated using version 3.01 of the CAMx air quality model using 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, 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 IVOC reductions required to compensate for INOx emission reductions.

Figure 4-7 displays the spatial distribution of daily maximum 1-hour ozone for the 2007 Strategy I8a scenario within the HGBPA 4-km modeling grid. Figure 4-8 displays the spatial distribution of daily maximum 1-hour ozone concentrations for the 200ole.200voc future year emission scenario, taking into account new source and ship emissions and with emission adjustments confined to the 8-county Houston-Galveston area. For completeness, the daily peak 1-hour ozone concentrations on the 4-km HGBPA domain for all the preliminary emission scenarios are presented in Table 4-3 and Table 4-4.

Table 4-3. Daily maximum ozone concentrations (ppb) for preliminary future year 2007 scenarios.

Scenario	09/08/93	09/09/93	09/10/93	09/11/93
i8 Base	156.5	145.2	149.2	150.9
i8 200ole 200voc	158.9	147.2	150.1	160.5
85nox 0voc	159.0	147.2	150.3	147.5
85nox 10voc	159.4	147.5	150.4	149.0
85nox 20voc	159.7	147.7	150.5	150.4
85nox 30voc	160.0	148.0	150.6	151.9
85nox 50voc	160.7	148.5	150.8	154.8
85nox 60voc	161.0	148.8	150.8	156.2
85nox 70voc	161.4	149.2	150.9	157.5
85nox 80voc	161.9	150.2	151.0	158.7
85nox 90voc	162.3	151.2	151.1	159.9
85nox 100voc	162.7	152.2	151.2	161.1
85nox 110voc	163.8	153.3	151.8	164.5
85nox 120voc	163.8	154.9	152.3	166.2
85nox 130voc	163.0	155.6	152.7	166.3
85nox 140voc	161.8	155.7	152.9	165.0
85nox 150voc	164.7	156.5	151.6	166.1
80nox 0voc	162.2	150.0	151.8	150.0
80nox 10voc	162.6	150.3	151.9	151.5
80nox 20voc	163.0	150.7	152.1	153.0
80nox 30voc	163.7	151.0	152.2	154.6
80nox 50voc	165.0	152.2	152.4	157.7
80nox 60voc	165.7	153.6	152.5	159.2
80nox 70voc	166.3	155.1	152.6	160.9
80nox 80voc	166.8	156.4	152.7	162.4
80nox 90voc	167.4	157.7	152.8	164.0
80nox 100voc	168.0	159.0	152.9	165.4

Scenario	09/08/93	09/09/93	09/10/93	09/11/93
80nox 110voc	168.6	160.3	153.0	166.8
80nox 120voc	169.2	161.5	153.1	168.2
80nox 130voc	169.7	162.6	153.2	169.5
80nox 140voc	170.3	163.8	153.3	170.8
80nox 150voc	170.9	164.9	153.4	172.0

Table 4-4. Daily maximum ozone concentrations (ppb) for preliminary future year 2007 scenarios changing olefins rather than total VOC.

Scenario	09/08/93	09/09/93	09/10/93	09/11/93
0.0ole 80nox	167.4	172.8	153.0	163.0
0.2ole 80nox	167.9	172.8	153.0	164.4
0.5ole 80nox	168.8	172.8	153.2	166.4
0.7ole 80nox	169.4	172.8	153.2	167.7
1.0ole 80nox	170.4	172.8	153.4	169.5
1.2ole 80nox	171.0	172.8	153.4	170.7
1.5ole 80nox	171.8	178.8	153.6	172.5
2.5ole 80nox	174.6	200.3	154.0	177.8
3.5ole 80nox	177.0	216.1	157.9	182.3
0.0ole 85nox	162.0	172.8	151.3	158.6
0.2ole 85nox	162.4	172.8	151.3	159.7
0.5ole 85nox	163.0	172.8	151.4	161.4
0.7ole 85nox	163.3	172.8	151.5	162.4
1.0ole 85nox	163.9	172.9	151.6	163.9
1.2ole 85nox	164.2	172.9	151.7	164.9
1.5ole 85nox	164.7	178.3	151.8	166.2
2.5ole 85nox	166.6	192.5	152.1	170.4
3.5ole 85nox	168.5	205.0	153.7	174.1

An examination of Figures 4-7 and Figure 4-8 reveals the effect of increased industrial VOC emissions on the daily peak ozone levels in the 2007 future year scenario. The spatial distributions are similar while the peak ozone concentration increases range from approximately 1 ppb in September 10th to as much as 10 ppb on September 11th. The locations of the daily maximum 1-hour ozone concentrations are the same for both simulations. The results displayed in Figure 4-8 represent the target to be reached to demonstrate equivalency between industrial NOx and VOC emission reductions.

In order to investigate the potential for compensating industrial NOx emission reductions with appropriate industrial VOC emission reductions, the industrial NOx emissions were "doubled" from the Strategy i8a levels. These adjustments were applied only to those sources within the 8-county Houston-Galveston region and only for those sources subject to control, as described above. These emission adjustments amount to a 71 ton per day increase in industrial NOx from the Strategy i8a control case. The industrial VOC emissions amount to 563 tons per day within the HGBPA 4-km domain. The results of this scenario, which includes doubled emission levels for industrial VOC and olefins, are presented in Figure 4-8, which displays the daily maximum 1-hour ozone concentrations on the HGBPA 4-km modeling domain. Note that these figures are based on the modeling results at 4-km resolution. The modeled peaks within the 1-33km grid may be somewhat higher. These simulation results represent the starting point for the investigation of compensating VOC emission reductions. In addition to the "doubled" industrial NOx scenario, corresponding to an 80% NOx reduction from the base year to the future year control case, a series of simulations also were investigated with an 85% NOx reduction level. The spatial distributions of peak 1-hour ozone concentrations for this case are shown in Figure 4-10.

A series of emission reduction scenarios were undertaken for both the 80% INOx and 85% INOx cases in which the industrial VOC emission levels were systematically reduced to determine a potential compensation level for the industrial NOx emission reductions. Figures 4-11 and 4-12 display the maximum potential ozone reductions which could be realized under each of these scenarios, i.e., with a 100% reduction of IVOC emissions. Potential ozone reductions are seen to be possible in localized regions within and downwind of the ship channel area and offshore. The daily maximum 1-hour ozone concentrations resulting from each of the emission reduction scenarios are tabulated in Table 4-5. Note that these peak concentrations are based on 1.33-km resolution over the 4-km HGBPA modeling domain while the displays are presented in terms of 4-km resolution results.

Table 4-5. Daily maximum ozone concentrations (ppb) in the 4-km HGBPA domain

Date/Time	9/8	9/9	9/10	9/11
90nox 200voc	159.0	175.2	150.1	160.8
80nox 0voc	159.1	172.8	149.8	147.8
80nox 50voc	160.7	172.8	150.2	155.1
80nox 100voc	162.7	172.8	150.7	161.5
80nox 150voc	164.7	175.0	151.1	166.6
80nox 200voc	166.9	189.6	151.4	170.8
85nox 0voc	158.2	172.8	149.2	146.3
85nox 50voc	158.6	172.8	149.6	152.8
85nox 100voc	159.8	172.8	150.0	158.2
85nox 150voc	161.1	172.8	150.4	162.6
85nox 200voc	162.5	183.1	150.8	166.2

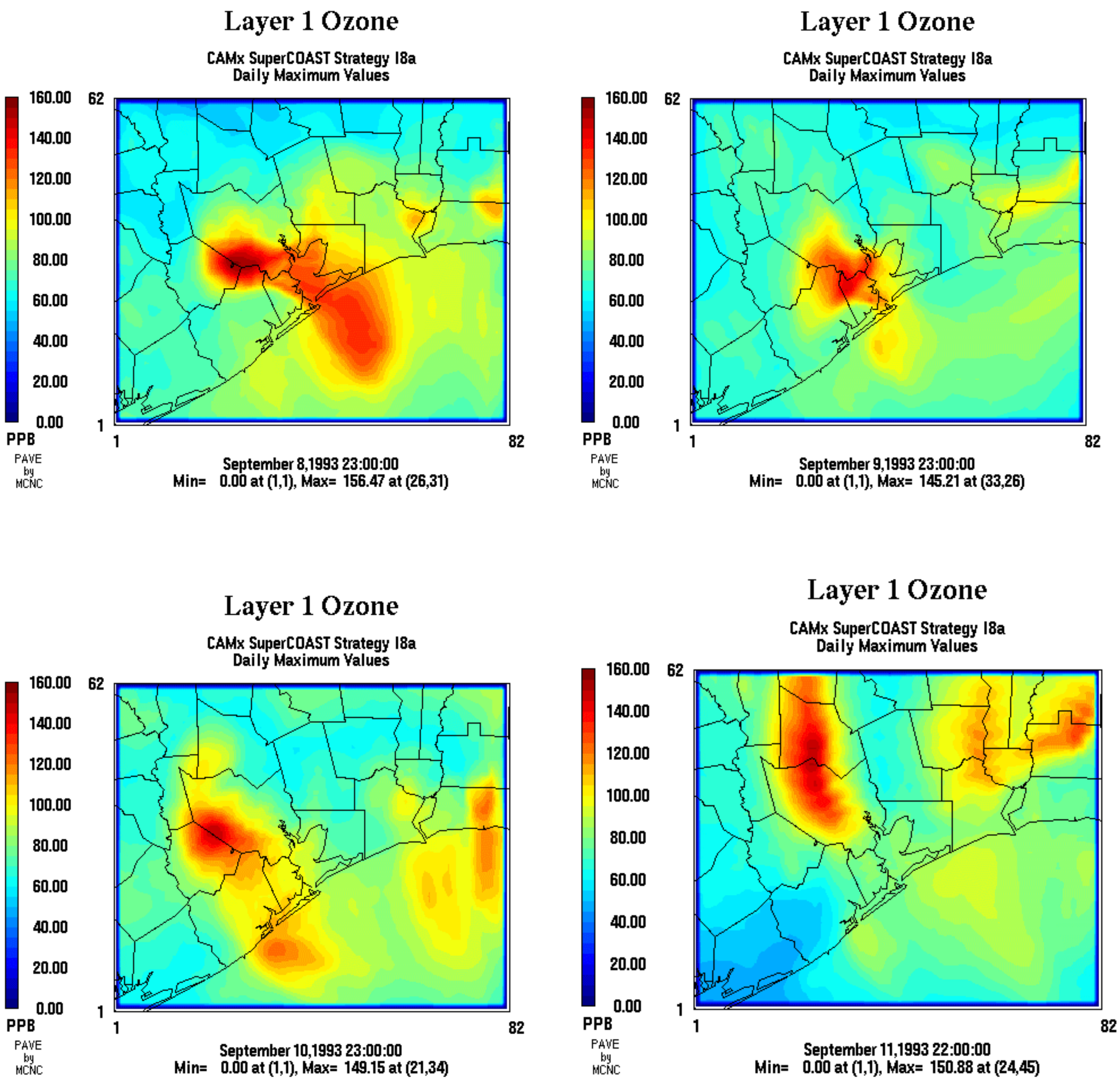


Figure 4-7. Daily maximum ozone for Strategy I8a on 4-km HGBPA domain.

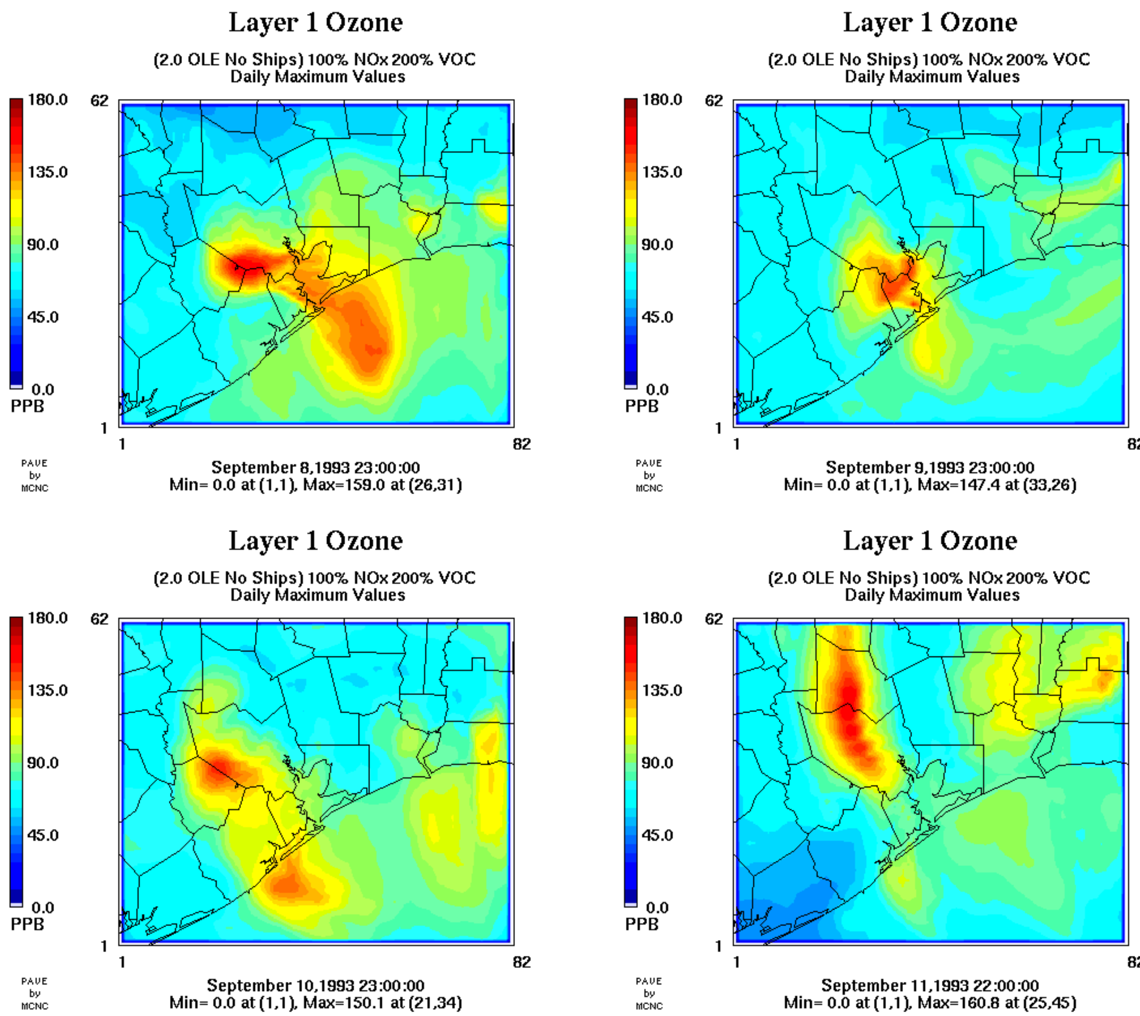


Figure 4-8. Daily Maximum Ozone with i8 NOx emission levels (90% reduction) and 200% VOC emissions levels and doubled olefins.

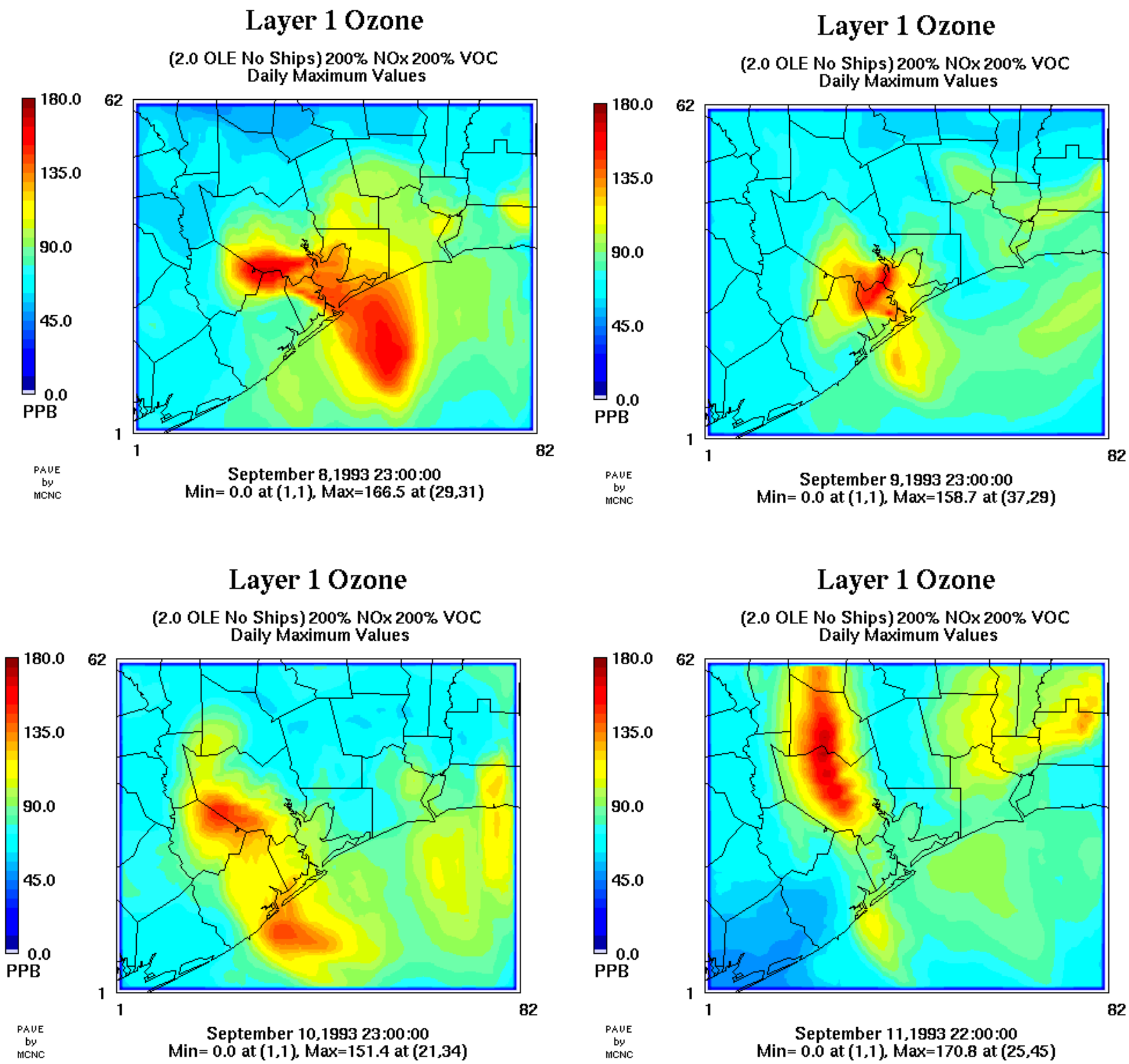


Figure 4-9. Daily Maximum Ozone with 200% i8 NOx emission levels (80% reduction) and 200% VOC emissions levels and doubled olefins.

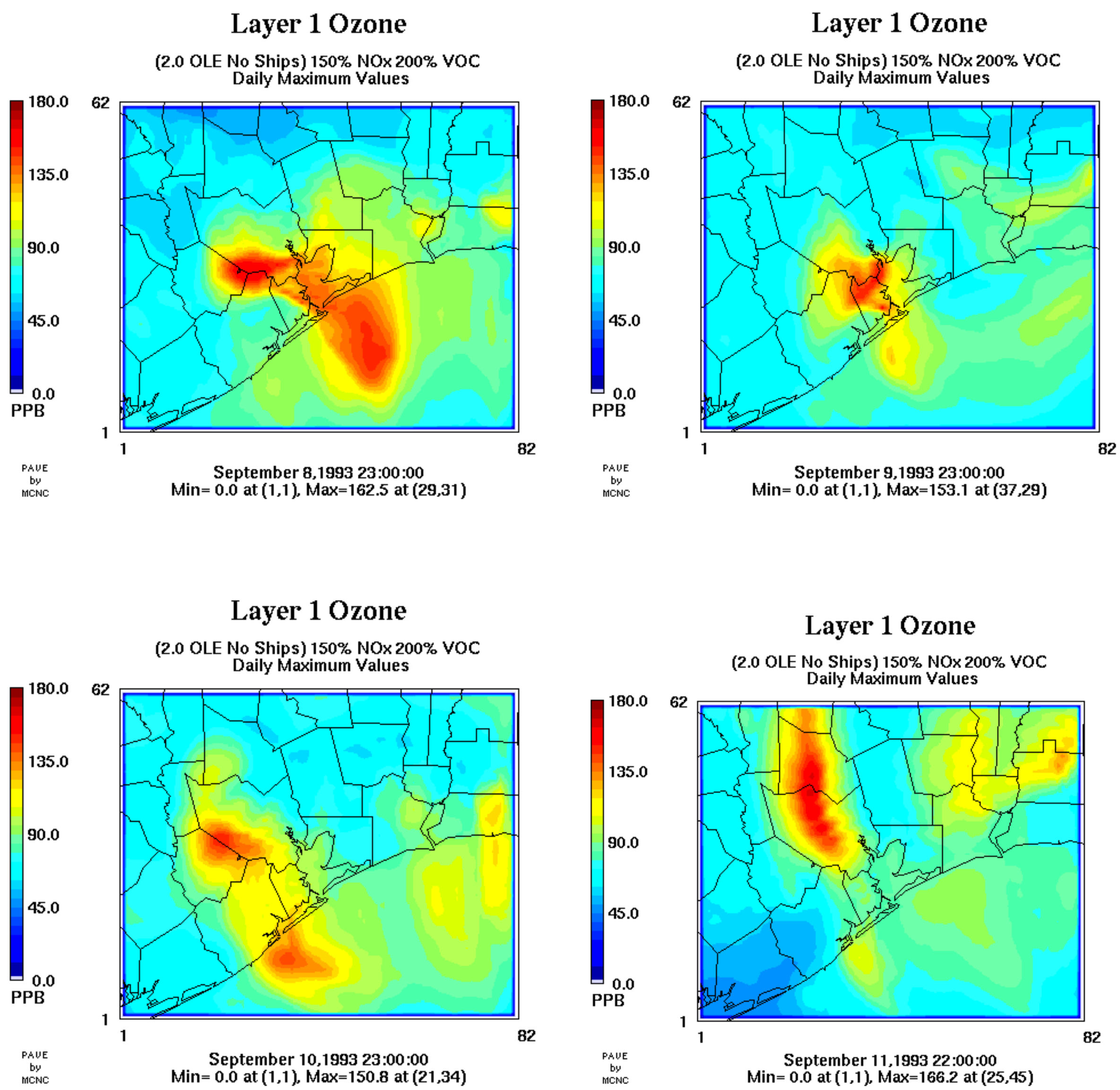


Figure 4-10. Daily Maximum Ozone with 150% i8 NOx emission levels (85% reduction) and 200% VOC emissions levels and doubled olefins.

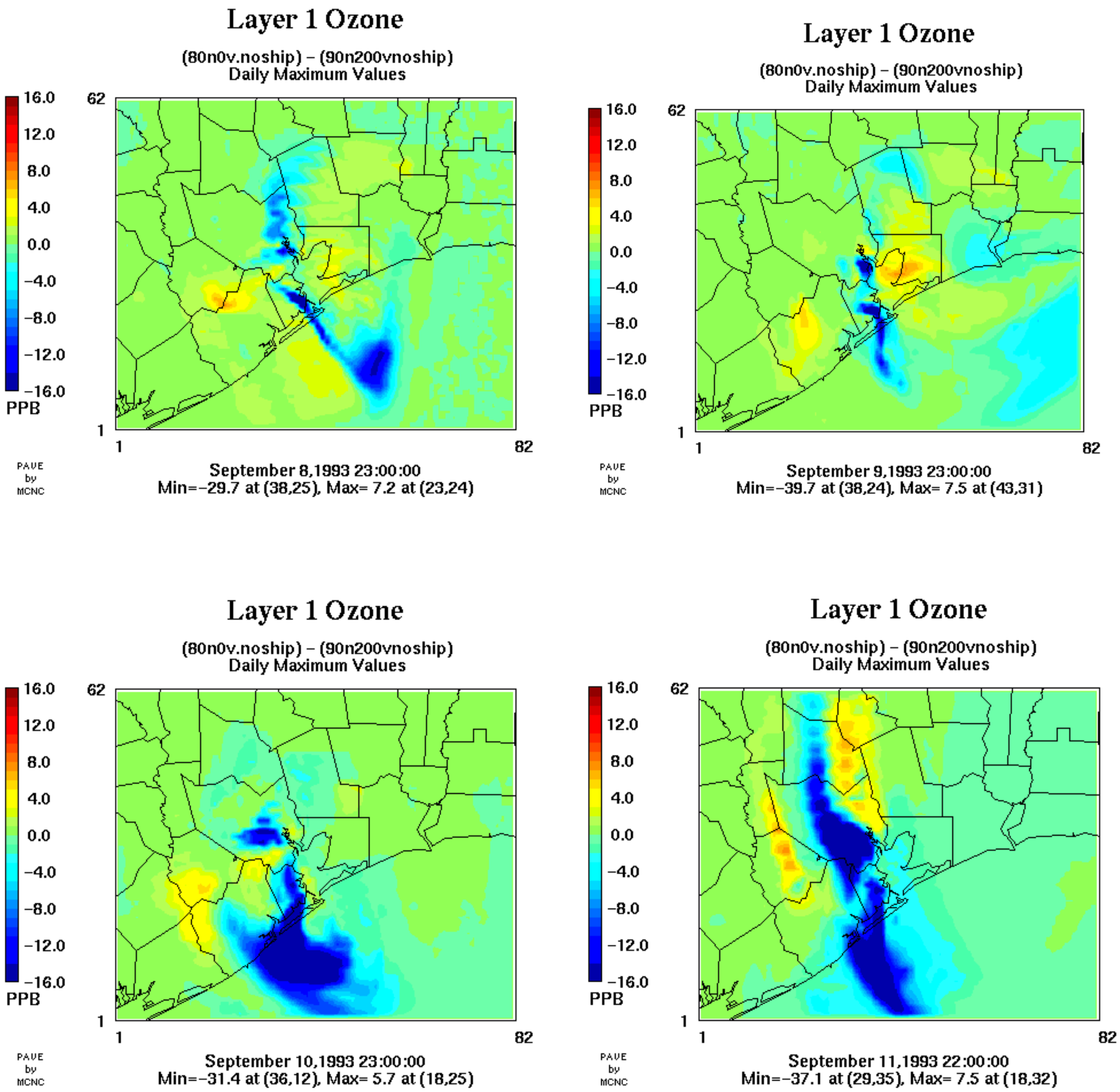


Figure 4-11. Maximum potential ozone reductions from the 200% i8 NOx emission levels (80% reduction) resulting from 100% reduction of IVOC emissions.

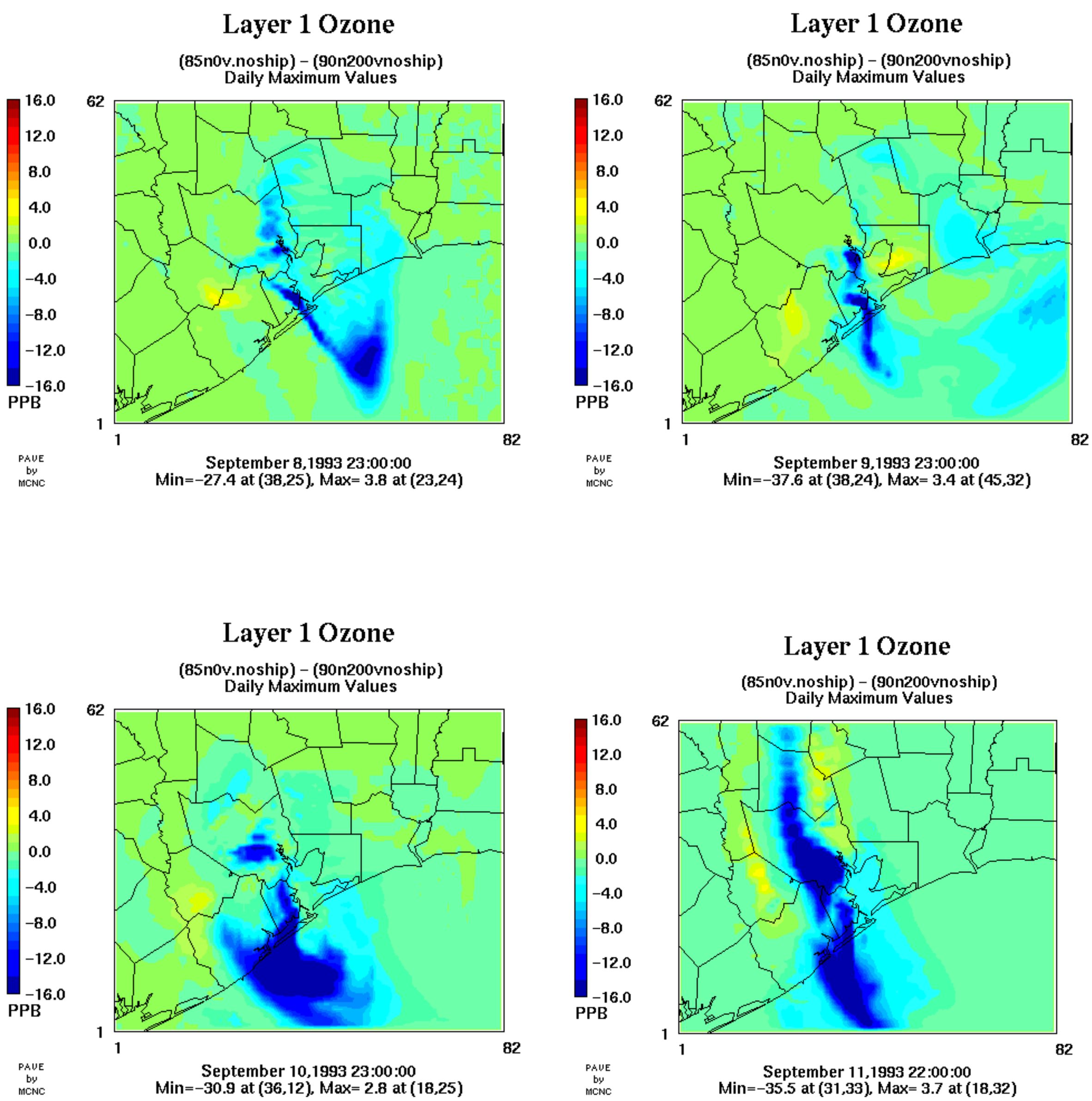


Figure 4-12. Maximum potential ozone reductions from the 150% i8 NOx emission levels (85% reduction) resulting from 100% reduction of IVOC emissions.

Figure 4-13 illustrates the effects of "doubled" industrial NOx emission and a 50% reduction of industrial VOC emissions. In general, broad regions of ozone increases within and downwind of the Houston Ship Channel are the result of increases in industrial NOx emissions. The increases in peak ozone concentrations range from approximately 7 ppb to over 9 ppb, depending on the simulation day. Decreases in daily maximum ozone concentrations are also realized, due to decreased industrial VOC emissions. These decreases tend to be somewhat localized and range from a 10.6 ppb decrease on September 8th to approximately 23 ppb on the 11th. These results serve to illustrate the trade-off between doubling industrial NOx emissions and halving industrial VOC emissions within the 8-county Houston-Galveston area and can be seen to vary considerably depending on the episode day. Qualitatively similar results are obtained for other VOC reduction levels as well as for the 85% industrial NOx series of simulations.

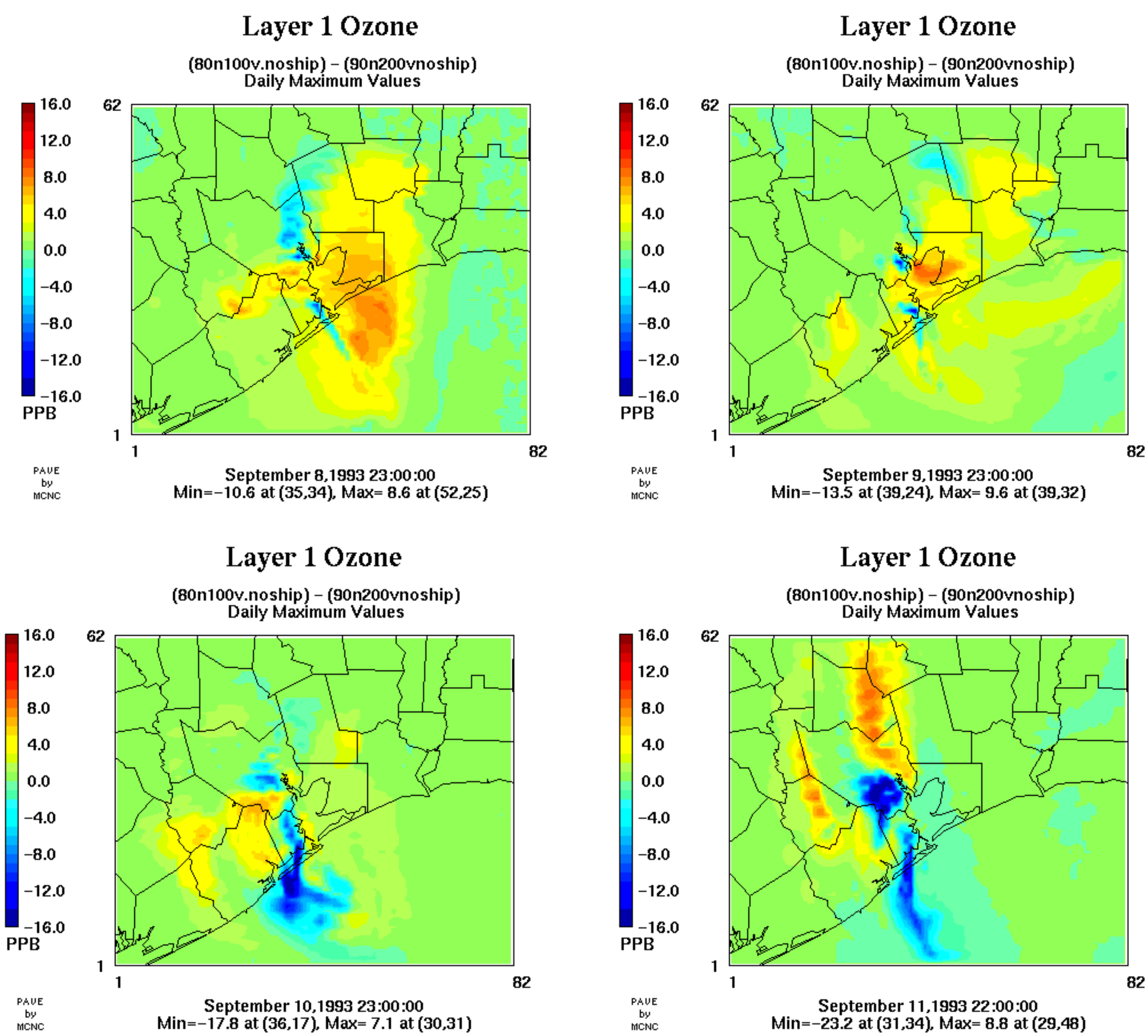


Figure 4-13. Effects of doubled industrial NOx emissions and 50% reduction of industrial VOC emissions on daily peak ozone concentrations.

A quantitative analysis of the sensitivity scenarios investigated is presented in Tables 4-6 and Table 4-7 for the 80% and 85% NOx emissions reduction series, respectively. A graphical representation of the analysis is displayed in Figure 4-14 and Figure 4-15. In Tables 4-6 and 4-7 the 90nox.200voc simulation represents the peak ozone concentration value which must be matched through reductions on industrial VOC emission levels. The 80nox.200voc simulation values provide the starting point for VOC emission reductions. The highlighted values in the Tables give the closest match obtained for the reduction scenarios considered. The necessary levels of VOC emission reductions required to compensate for industrial NOx emission reductions varies depending on the episode day.

As an example, on the September 8th episode day, doubling the industrial NOx emissions increases the peak ozone concentration in the 4-km HGBPA domain from 159.0 ppb to 166.9 ppb. Subsequent reduction of IVOC emission levels to zero brings the peak ozone level down to 159.1 ppb. Therefore, for this day, NOx emission reductions in the future year control case can only be compensated for with a 100% reduction in industrial VOC emissions. The analysis for the other simulation days is similar resulting in the following IVOC emission reduction levels required to compensate for doubling industrial NOx emissions: 100% on September 8th; ~25% on September 9th; ~75% on September 10th; and, ~50% on September 11th.

Table 4-6. INOx/IVOC Equivalence at the 80% NOx emissions level

Date/Time	**90nox 200voc**	**80nox 0voc**	**80nox 50voc**	**80nox 100voc**	**80nox 150voc**	**80nox 200voc**
9/8 Max	159.0	159.1	160.7	162.7	164.7	166.9
9/9 Max	175.2	172.8	172.8	172.8	175.0	189.6
9/10 Max	150.1	149.8	150.2	150.7	151.1	151.4
9/11 Max	160.8	147.8	155.1	161.5	166.6	170.8

Repeating the analysis for the 85% NOx emission level scenarios gives the following VOC emission reductions necessary for each day: ~75% on September 8th; ~25% on September 9th; ~50% on September 10th; and, ~25% on September 11th.

Table 4-7. INOx/IVOC Equivalence at the 85% NOx emissions level

Date/Time	90nox 200voc	85nox 0voc	85nox 50voc	85nox 100voc	85nox 150voc	85nox 200voc
9/8 Max	159.0	158.2	158.6	159.8	161.1	162.5
9/9 Max	175.2	172.8	172.8	172.8	172.8	183.1
9/10 Max	150.1	149.2	149.6	150.0	150.4	150.8
9/11 Max	160.8	146.3	152.8	158.2	162.6	166.2

Figures 4-14 and 4-15 display these relations graphically and provide a means for interpolating the results to other VOC emission reduction levels. These figures display the modeled peak ozone concentration as a function of the industrial VOC 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 double industrial VOC and olefin emissions. The intersection of the curves gives the required level of VOC emission reductions to compensate for the industrial NOx emission reductions for each day of the episode. The response of the modeled ozone peaks due to industrial VOC emission reductions can be seen and varies depending on the episode day.

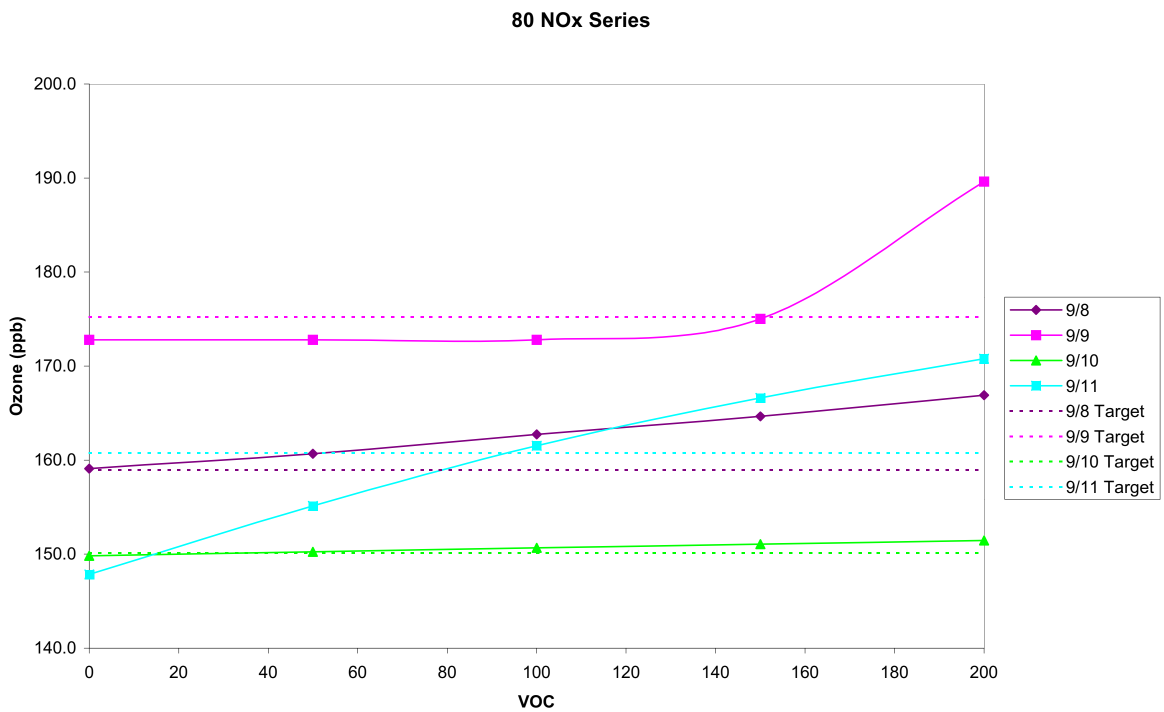


Figure 4-14. Graphic representation of INOx/IVOC equivalency for the 80% INOx series.

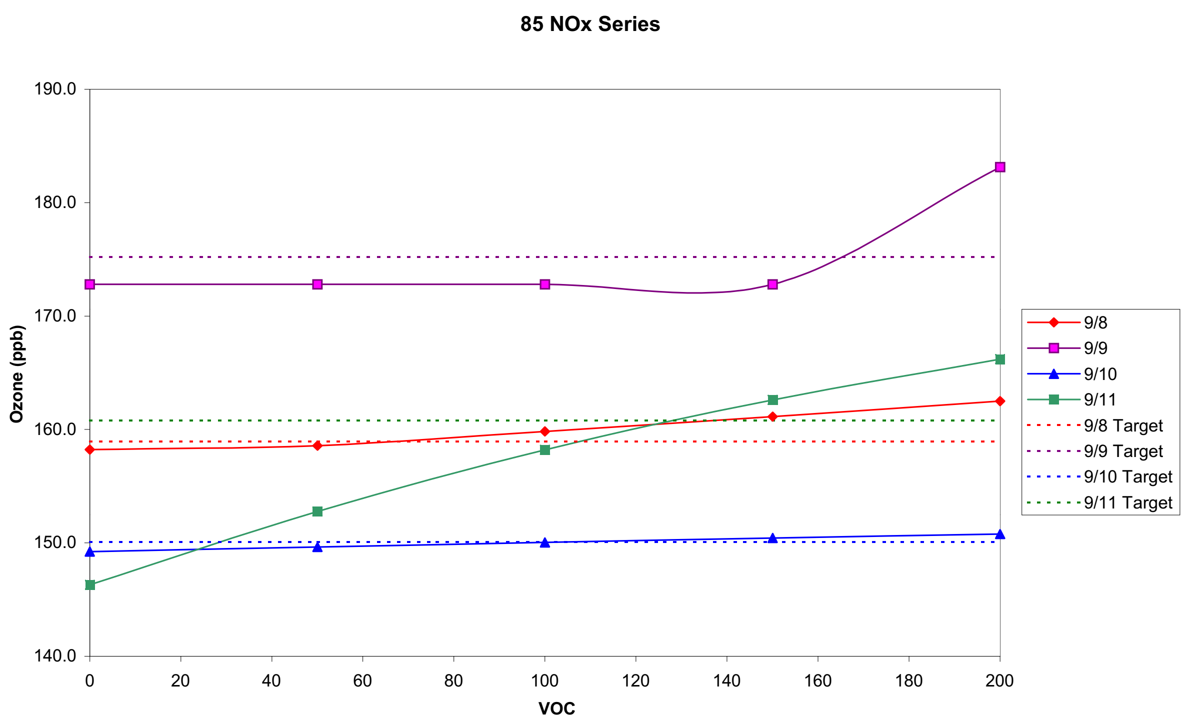


Figure 4-15. Graphic representation of INOx/IVOC equivalency for the 85% INOx series.

As with the 1993 Base Year simulations, a number of episodic VOC emission scenarios were investigated for the 2007 future year control case. Figure 4-15 displays the result of the UPSET1C scenario in terms of impacts on ozone concentrations. The first frame of Figure 4-16 displays the ozone impacts at 10:00am on September 8th, which corresponds to the maximum ozone difference between the upset conditions and future year base case. The second frame displays the impacts on the daily peak 1-hour ozone concentrations. While the impacts are not as large as was the case for the base year, the results confirm the ability of the CAMx model to replicate episodic high ozone events within the area of the Houston Ship Channel and Galveston Bay.

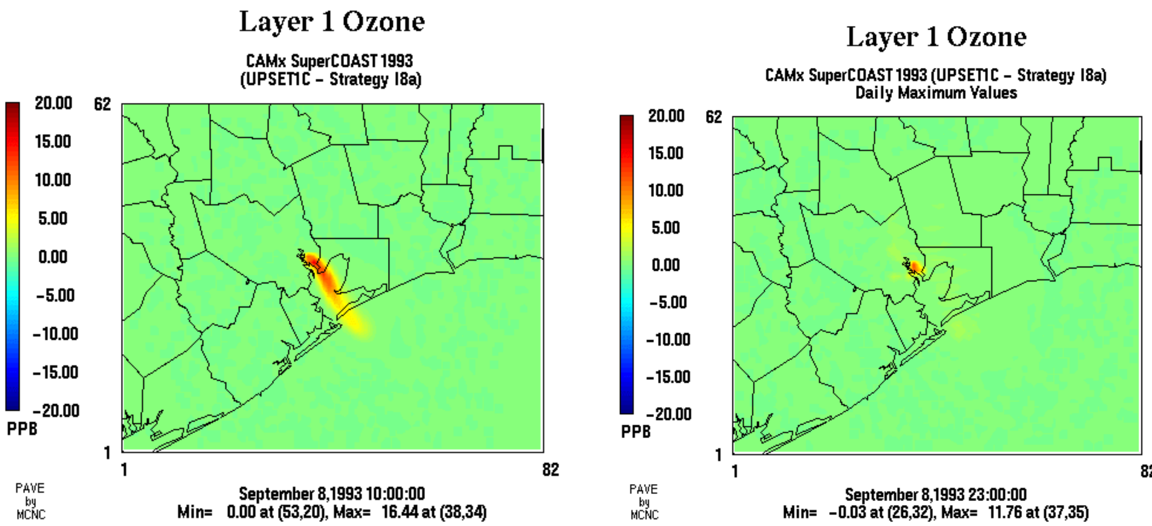


Figure 4-16. Future year ozone impacts due to UPSET1C scenario at 10 am September 8, 1993 and impacts on daily maximum 1-hour ozone.

Artificial Wind Experiments

At the direction of the TNRCC Project Manager, a number of additional highly experimental scenarios were investigated. The experimental scenario documented here was designed to assess the effect of industrial NOx and VOC emission reductions under conditions of unidirectional wind flow of constant magnitude. The purpose of the experiment is to evaluate the effects of partially segregating industrial emissions from the main body of urban emissions, allowing the evaluation of industrial control strategies with significantly reduced influence of pollutant contaminants from urban sources.

The experiment design consisted of unidirectional winds from due south at a constant speed of 2.5 m/s. Other meteorological inputs were unchanged from those of the SuperCOAST simulation data sets. Thus, temperature, pressure and vertical exchange coefficients from the original SAIMM based fields are paired with unrelated constant winds. Emissions data were based on the 2007 Strategy i8a control case. Industrial NOx and VOC emission adjustments were considered in the same manner as those previously described. Thus, starting with the 90% industrial NOx emission reductions of the Strategy i8a case, industrial olefins were first doubled, then industrial VOC were doubled, resulting in an overall 4 times increase in olefin emissions. This provided the target for compensating industrial VOC emission reductions.

As with the previously investigated emission reduction scenarios, the industrial NOx emission were "doubled" to provide an 80% NOx reduction level from the uncontrolled future year case. This resulted in an increase of 71 tons of NOx emissions in addition to an increase of industrial VOC emissions of approximately 563 tons. A series of VOC reduction scenarios were then undertaken wherein the VOC emission were decreased from the 200% level to 0% in increments of 50%, to determine the level of VOC emission reductions required to compensate for the increase in industrial NOx emission levels. The results of these experimental simulations are described here. The results of these experiments are linked to the "artificial winds" assumption and should be interpreted accordingly.

Figure 4-17 displays the original SAIMM surface winds as used in the SuperCOAST modeling and the artificial winds, both for reference and comparison and as a means of quality assurance of the wind fields. Displayed are the surface layer vector wind fields and isopleth plot of surface layer wind speeds for 12 noon on September 8th.

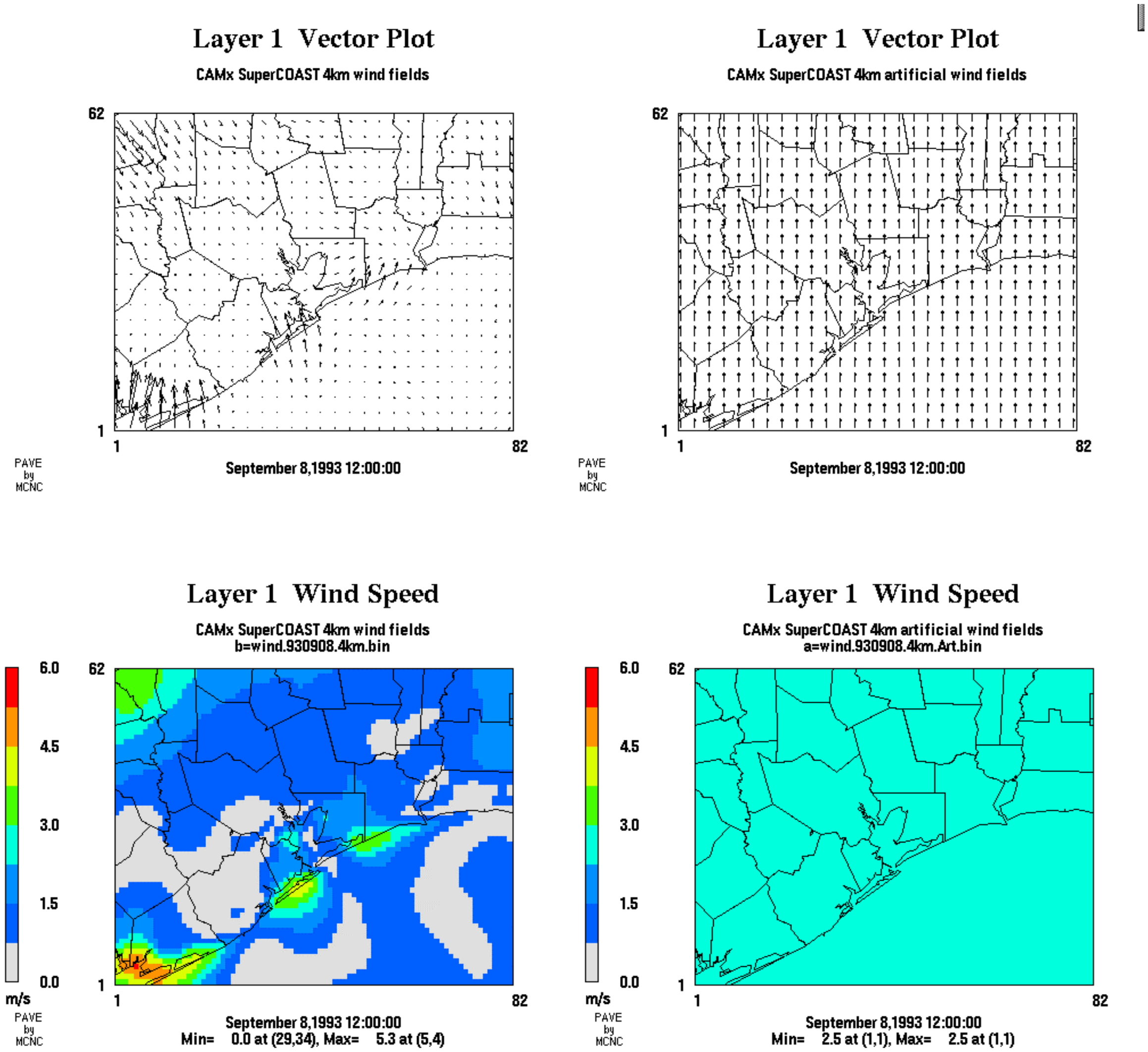


Figure 4-17. Comparison of SAIMM and artificial wind fields at 12 noon, September 8, 1993.

The daily maximum 1-hour ozone concentrations on the 4-km and 1.33-km domains are displayed in Figure 4-18 and Figure 4-19, respectively, for the 90% industrial NOx reduction (Strategy i8a) level and 200% industrial VOC and doubled olefins. As with the final series of alternative emission scenarios described previously, the emission adjustments performed for this experiment considered only those sources subject to controls and are confined to the 8-county Houston-Galveston area. For reference, Table 4-8 presents the daily peak ozone concentrations in the HGBPA 4-km modeling domain and the 1.33-km Houston modeling domain for the 90% NOx reduction; 200% VOC increase scenario.

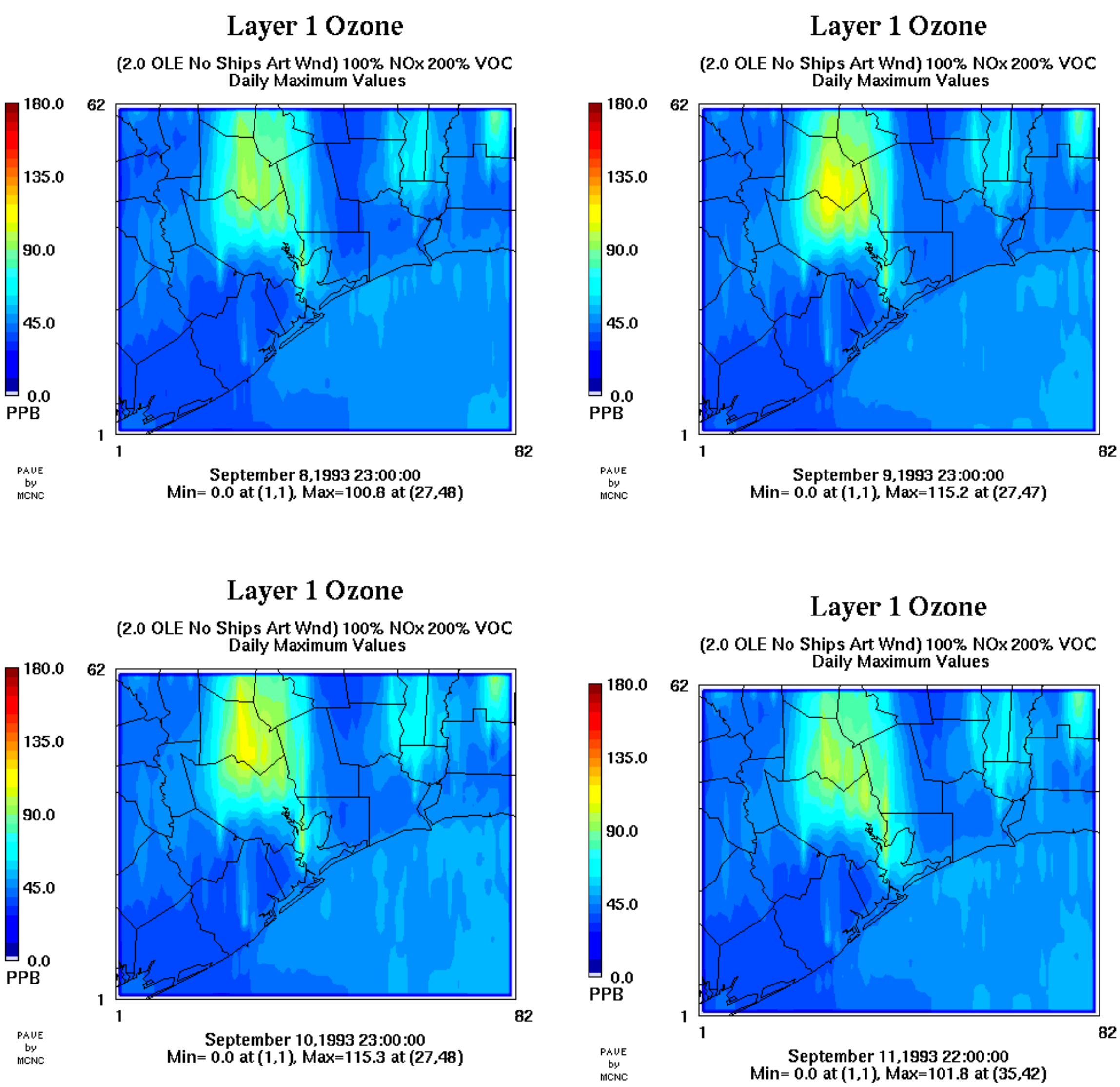


Figure 4-18. Daily Maximum Ozone with i8 NOx emission levels (90% reduction) and 200% VOC emissions levels and doubled olefins for the artificial wind experimental scenario on the 4-km domain.

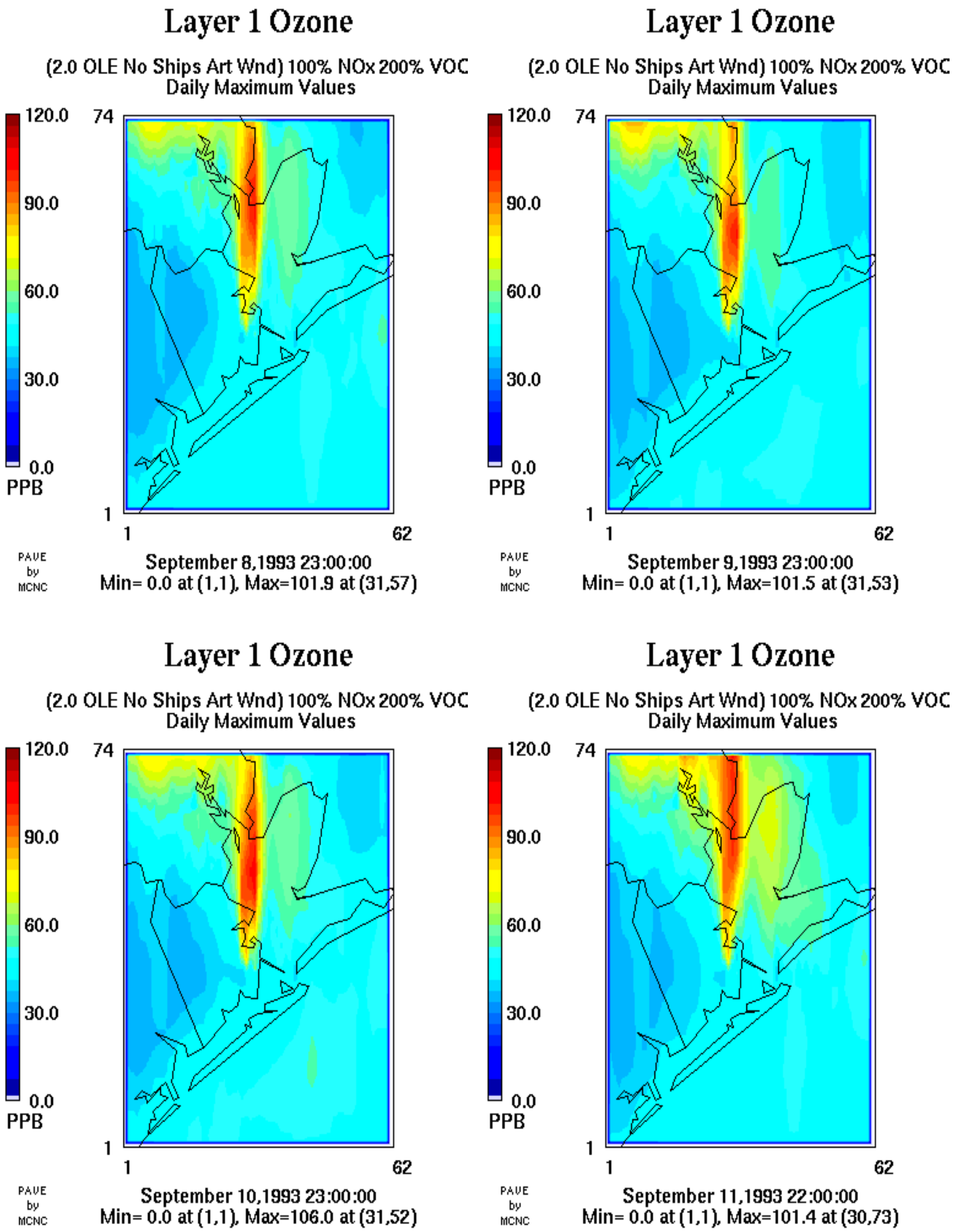


Figure 4-19. Daily Maximum Ozone with i8 NOx emission levels (90% reduction) and 200% VOC emissions levels and doubled olefins for the artificial wind experimental scenario on the 1.33-km domain..

Table 4-8. Daily maximum ozone concentrations (ppb) for i8a NOx levels and 200% VOC emission levels.

Date	Peak ozone (ppb) over the 1.33 km and 4 km grids with 90% NOx reduction and 200% VOCs	Peak ozone (ppb) over the 1.33 km grid with 90% NOx reduction and 200% VOCs
8-Sep	100.8	101.9
9-Sep	115.2	101.5
10-Sep	115.3	106.0
11-Sep	101.8	101.4

The effect of changes in industrial emissions within the 4-km and 1.33-km domains on September 9th are illustrated in Figure 4-20 and Figure 4-21. Figure 4-20 displays the difference in daily maximum 1-hour ozone concentrations due to decreasing industrial NOx reductions from 90% to 80% at the 200% VOC emission levels. These emission adjustments amount to a 71 ton per day increase in industrial NOx from the Strategy i8a control case. The industrial VOC emissions amount to 563 tons per day within the HGBPA 4-km domain. In the figure, the left panel presents the modeling results on the 4-km domain while the right panel presents the 1.33-km modeling results. The corresponding ozone peaks for the industrial VOC emissions at the100% level (281.5 tpd VOC emission decrease from “doubled” level) are displayed in Figure 4-21. The maximum potential ozone reductions which can be realized with “doubled” industrial NOx emissions and 100% VOC emission reduction (i.e., zero-out all industrial VOC emissions) are presented in Figure 4-22, which displays the difference in daily peak ozone concentrations in the 4-km and 1.33-km modeling domains.

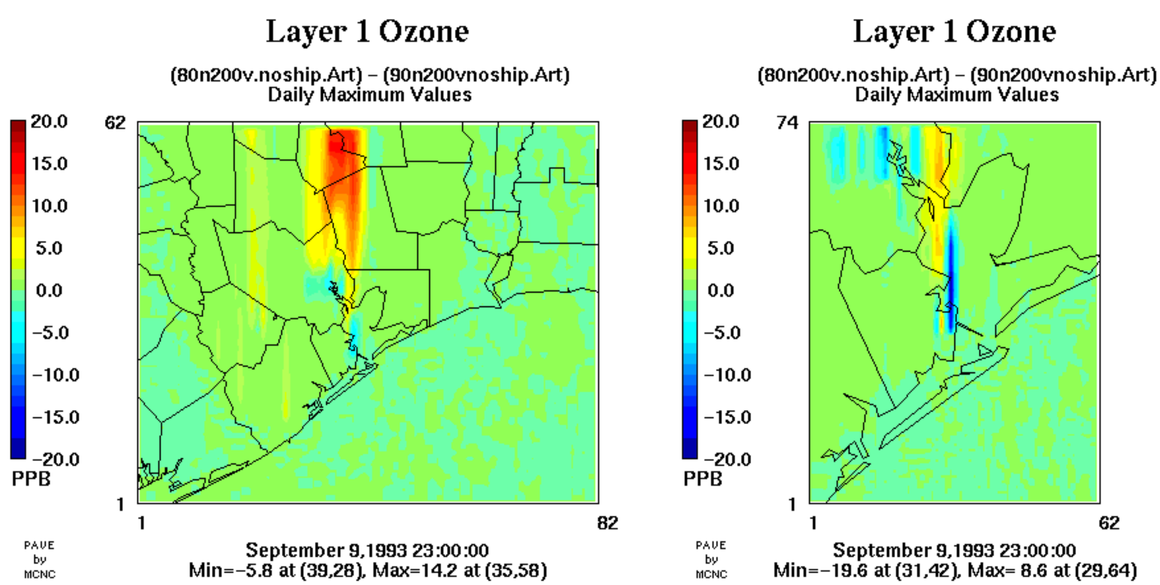


Figure 4-20. Effects of doubled industrial NOx emissions at 200% VOC emission levels on the daily maximum ozone concentrations for the artificial wind scenario.

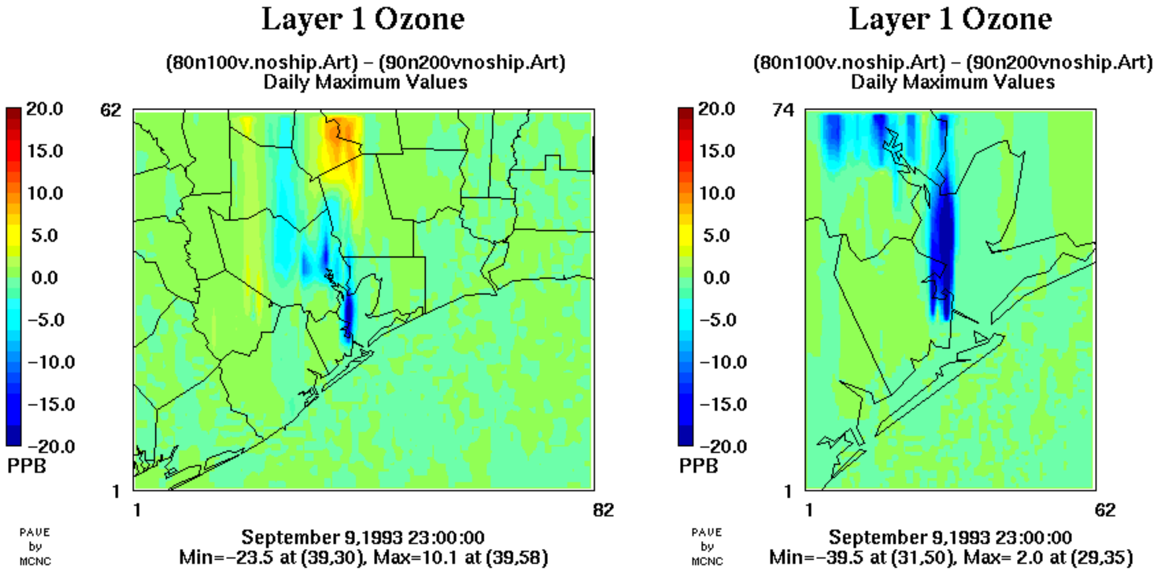


Figure 4-21. Effects of doubled industrial NOx emissions and 50% reduction of industrial VOC emissions on the daily maximum ozone concentrations for the artificial wind scenario.

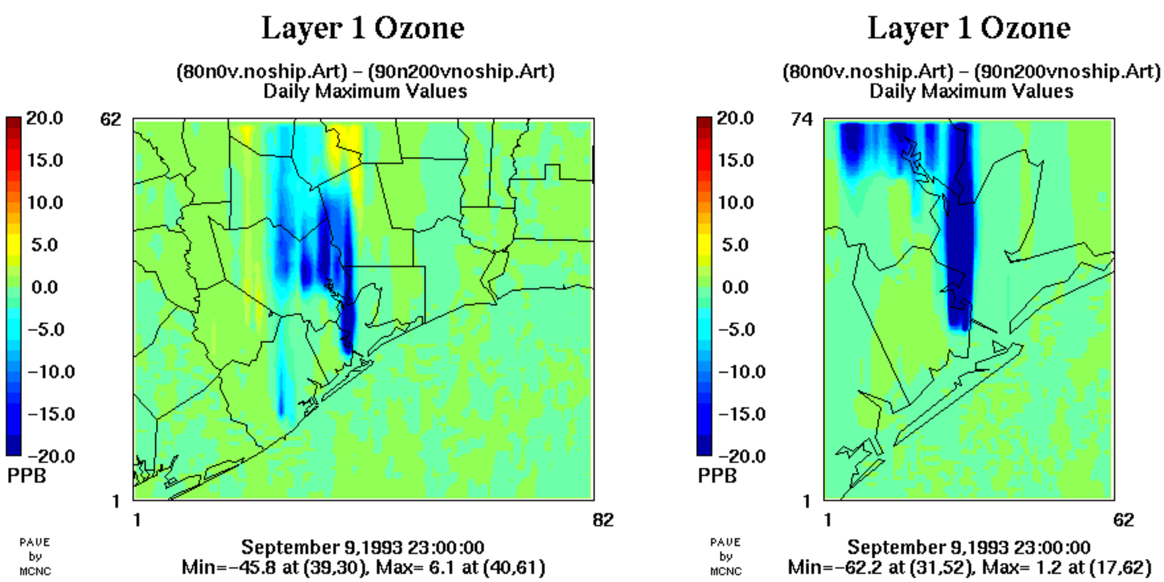


Figure 4-22. Maximum potential ozone reductions from the 200% i8 NOx emission levels (80% reduction) resulting from 100% reduction of IVOC emissions.

Table 4-9 presents the daily peak ozone concentrations for the artificial wind experiment simulations and an analysis of the equivalence between industrial NOx and VOC emission reductions. In the table, 90nox.200voc represents the "i8a base case" with doubled olefins and doubled VOC emissions, while the 80nox indicates an 80% NOx reduction level from the uncontrolled future year case, i.e., a 71 ton increase from the 90nox scenario. The 200voc indicates doubled industrial VOC emissions, which amount to 563 tons per day of industrial VOC, and 0voc represents zero tons of industrial VOC.

Table 4-9. Daily maximum ozone concentrations (ppb) for the artificial wind experiment emission scenarios.

Date	90nox 200voc	80nox 200voc	80nox 150voc	80nox 100voc	80nox 50voc	80nox 0voc
8-Sep	101.9	103.9	100.4	98.5	97.0	95.7
9-Sep	115.2	115.7	113.4	110.8	108.0	105.5
10-Sep	115.3	115.7	114.0	112.2	110.2	108.2
11-Sep	101.8	111.3	105.3	99.1	97.5	95.7

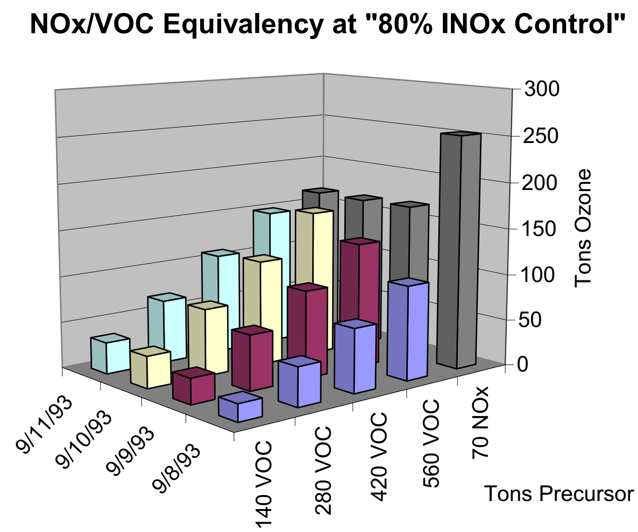
The following observations can be made from the results presented in Table 4-7. Increasing the NOx emission from industrial source in the Houston Ship Channel area increases the ozone peaks. Relaxing NOx controls from 90% reduction to 80% reduction increases the daily peak ozone concentrations 0.4 to 9.5 ppb, depending on the episode day. A decrease in industrial VOC emissions results in decreases in the ozone peaks. A 25% reduction in industrial VOC emissions (200voc to 150voc) reduces peak ozone levels 1.7 to 6 ppb while a 50% VOC reduction (200voc to 100voc) results in ozone peak reductions from 3.6ppb to 12.2 ppb, depending on the episode day.

Process Analysis

Process analysis was conducted with the various emission control scenarios to provide some additional insight to the NOx/VOC equivalency. Based on the mass budget diagnostic output provided by the CAMx model, the amount of ozone produced through chemical processes as well as the corresponding amount of NOx and VOC emissions were analyzed for each of the emission scenarios. The procedures involved calculation of the tons of NOx, VOC and ozone on a domain-wide basis and balancing changes in total ozone production between increases in industrial NOx emissions and decreases in industrial VOC emissions.

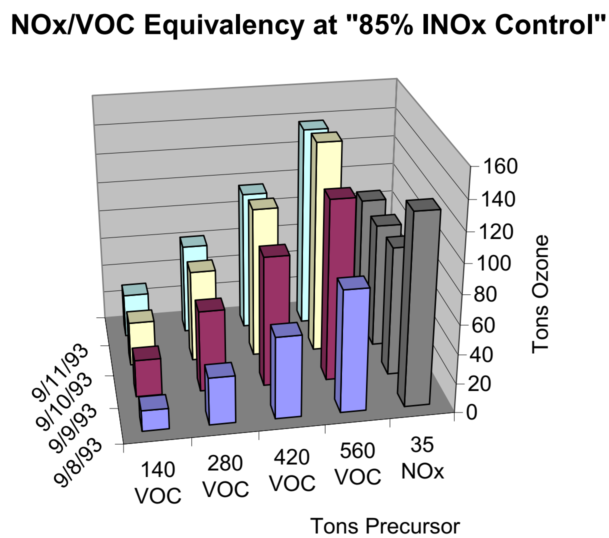
Figures 4-23, 4-24, and 4-25 provide a graphical illustration of the NOx/VOC equivalency for the various emission scenarios for the 80% NOx levels, the 85% NOx levels, and the 80% NOx levels for the artificial wind experiments, respectively. In the figures, the increase in tons of ozone produced at the various increased industrial NOx emission levels are displayed for each episode day. The data used in the analysis are presented in the tables below each figure. Also displayed are the corresponding tons of ozone produced due to varying industrial VOC emission levels. The equivalency between NOx and VOC emissions on ozone production is obtained when the amount of ozone due to industrial VOC emissions is equal to the amount of ozone production due to industrial NOx emission.

An examination of the figures reveals the dependence of the NOx/VOC equivalence by episode day. Figure 4-23 illustrate the results of the 80% industrial NOx emission levels and highlights the findings that for most days the increase in NOx emission can not be balanced by industrial VOC emission reductions. The results of the 85% NOx emission scenarios, shown in Figure 4-24, illustrate the potential for compensating NOx emission reductions with industrial VOC emission reductions is promising for all episode days except Sept. 8th . It is worth noting that the response is approximately linear with VOC emission reductions and therefore interpolation, or extrapolation, between the various VOC emission reduction levels is possible. Figure 4-25 displays the results of the process analysis for the artificial wind experimental scenarios. As in the 85% NOx emission series, NOx/VOC equivalence is possible for a number of VOC emission reduction levels.



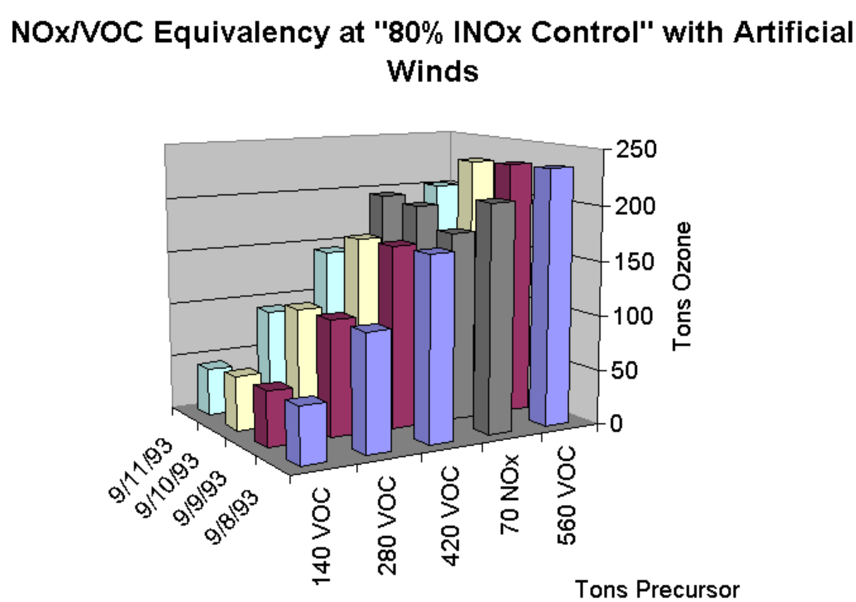
	140 VOC	280 VOC	420 VOC	560 VOC	70 NOx
9/8/93	19	42	68	101	252
9/9/93	27	59	94	134	167
9/10/93	34	72	114	159	166
9/11/93	34	68	109	149	165

Figure 4-23. Process Analysis results for the 80% industrial NOx emission level scenarios.



	140 VOC	280 VOC	420 VOC	560 VOC	35 NOx
9/8/93	14	32	56	83	130
9/9/93	25	55	89	123	88
9/10/93	30	63	103	145	85
9/11/93	30	62	96	138	86

Figure 4-24. Process Analysis results for the 85% industrial NOx emission level scenarios.



	140 VOC	280 VOC	420 VOC	70 NOx	560 VOC
9/8/93	51	107	167	207	234
9/9/93	50	106	166	173	232
9/10/93	50	105	164	191	230
9/11/93	44	92	144	195	201

Figure 4-25. Process Analysis results for the 80% industrial NOx emission level scenarios for the artificial wind experiments..

5. SUMMARY

The CAMx air quality model was applied to the September 8-11, 1993 ozone episode on the SuperCOAST domain. Based on the findings of Task 2 of this Work Assignment, version 3.01 of the CAMx model with chlorine chemistry was implemented. A flexi-nested 1.33-km 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. 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. In addition, a number of episodic emission scenarios were developed to characterize the types of non-routine emission levels known to occur in the industrial areas around Houston and model simulations performed to assess the sensitivity of model performance to these emission adjustments.

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.

Finally, a number of additional experimental scenarios were investigated. These scenarios were designed to evaluate the effects of partially segregating industrial emission from the main body of urban emissions, allowing an evaluation of industrial control strategies with reduced influence of pollutants from urban sources.

The following conclusions can be drawn from the model simulations performed for this study:

- Based on the analysis of the alternative industrial VOC emission scenarios, the 200ole.200voc 1993 base year simulation (doubled olefins and double VOC emission levels) provides acceptable model performance with respect to EPA guidance on model performance goals. As this scenario provides a level of pollutants within the Houston-Galveston area, consistent with the findings of the 2000 TexAQS, it was selected as the basis of future year control scenario simulations.

- The results of the non-routine (upset conditions) and episodic VOC emission scenarios indicate that the CAMx model is capable of providing a reasonable representation of events leading to episodic elevated ozone concentrations within the industrial areas of the Houston Ship Channel and Galveston Bay.

- An analysis of the alternative emission scenarios for the future year control case demonstrates 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 VOC emission reductions has been shown to be theoretically possible for some episode days at the 80% NOx emission levels with varying VOC emission reductions, albeit extremely large VOC emission reductions in most cases. For the 85% NOx emission reduction levels, compensation potential again varies by day and, except for the September 8th episode day, compensating NOx emission reductions with VOC emission reductions would be possible at a number of VOC 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 VOC emissions produce more localized ozone reductions.

- The results of the artificial wind experiment simulations attempt to illustrate the efficacy of industrial control strategies with significantly reduced contamination from urban emission sources. The unidirectional wind fields have the effect of partially segregating the industrial emission from the main body of urban emissions and the analysis shows an increased potential for offsetting NOx emission reductions with industrial VOC emission 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 result presented here.

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