APPENDIX D

Development of the SuperCOAST Modeling Setup

Houston/Galveston Attainment Demonstration and
Post-1999 Rate-of-Progress SIP

December 2000

MIGRATION TO THE REGIONAL SUPERCOAST DOMAIN AND TO CAMX VERSION 2

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1. INTRODUCTION

The Coastal Oxidant Assessment for Southeast Texas (COAST) modeling domain (Figure 1) has been used for most State Implementation Plan (SIP) modeling activities for the state of Texas. However, a larger, regional scale domain was used to generate boundary and initial conditions for the COAST domain. This regional scale domain (Figure 2) consists of one grid at a 16km horizontal resolution. The Texas Natural Resource Conservation Commission (TNRCC) tasked MCNC with combining the regional and COAST domains into a new regional modeling domain to be called the Super Coastal Oxidant Assessment for Southeast Texas (SuperCOAST) modeling domain. The purpose of this project was to replace two model runs - one throughout the regional domain to generate boundary conditions for a second model run on the COAST domain - with one model run utilizing the 4 km COAST domain as a nest within the regional 16 km domain. This effort would include combining air quality modeling input data from both domains as well as generating new input data. The Comprehensive Air Quality Model with Extensions (CAMx) version 1.13 had been used in most recent modeling effort for both the COAST and regional modeling domains. TNRCC also tasked MCNC to migrate from CAMx version 1.13 to version 2. MCNC would recalculate performance statistics to examine any change in performance over the Houston-Galveston non-attainment area. This report summarizes the steps taken to complete migration to the SuperCOAST domain and to CAMx version 2 for the September 6-11, 1993 episode.

Houston–Galveston Modeling Domain

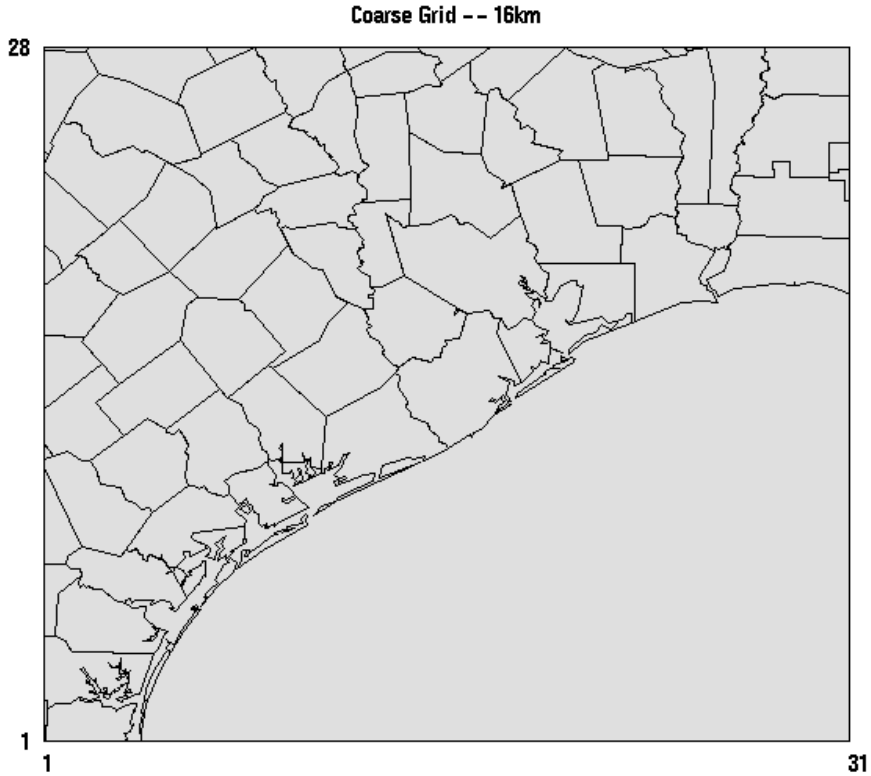

Figure 1. COAST 16km horizontal resolution modeling domain.

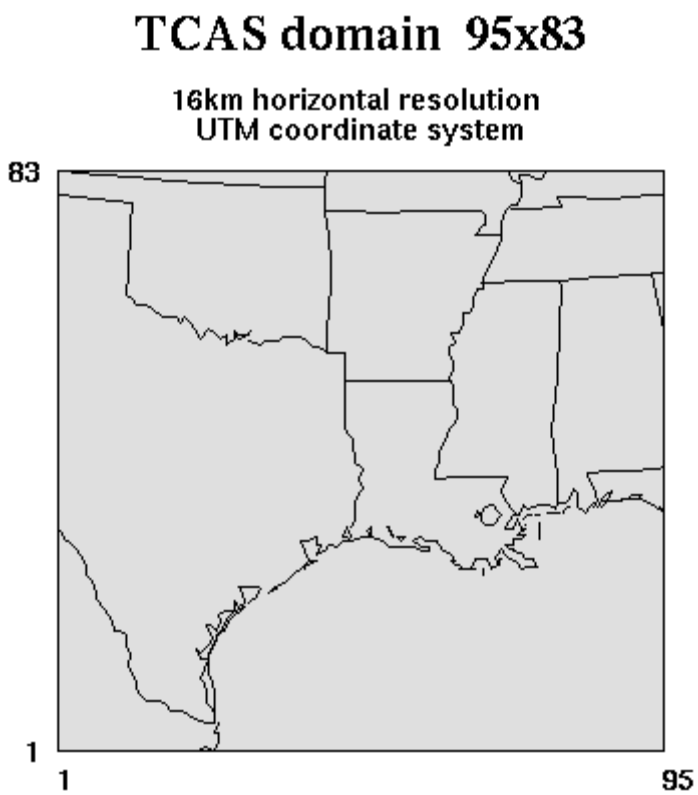

Figure 2. Regional 16 km resolution modeling domain.

2. METHODOLOGY

MCNC acquired from TNRCC CAMx input data for the regional domain for the September 6-11, 1993 episode. MCNC developed a program that substituted the COAST 16 km resolution data for the regional 16 km resolution data over the COAST portion of the SuperCOAST domain. Data on 4km COAST points was unchanged. Quality assurance was performed using the Package for Analysis and Visualization of Environmental data (PAVE) on the resulting SuperCOAST data to ensure proper substitution of data. This substitution was carried out on the following input files:

- WIND: 3-dimensional wind fields
- H2O: 3-dimensional water vapor fields
- KV: 3-dimensional vertical diffusion coefficients
- TEMP: 3-dimensional temperature fields
- LANDUSE: 2-dimensional land use data
- EMISSIONS: 2-dimensional low-level emissions data

The other input data that needed to be modified for SuperCOAST modeling included:

- RATES: Photolysis rates
- AHZOZ: Albedo, haze, and ozone column file

The modifications were made at TNRCC and MCNC to better estimate these variables when using the SuperCOAST grids. No modifications were made to the 4 km nested grid input files.

The migration to CAMx version 2 required the use of a new chemistry parameters (CHEMPARAM) file. Also, WIND and TEMP files required an extra hour of data for each simulation day. Each simulation day has 24 hours worth of data in CAMx version 1.13 modeling. MCNC used a program to copy the hour 24 data to an additional hour 25 to meet this CAMx version 2 requirement.

3. CAM$_X$ SETUP

An example of the CAMx version 2 script can be found in Appendix A. The regional simulations done at TNRCC consisted of running September 5-11, 1993. The SuperCOAST domain runs consisted of running September 5 with generally the same input data used by TNRCC but instead using CAMx version 2. Note that there is no 4 km nested grid on September 5th, so the average concentration file from the September 5th CAMx version 2 had to be used as the initial conditions for September 6th. On September 6th, the 4 km nested grid is introduced and is generally treated as a cold start. Also, note that CAMx version 2 supports the use of fine grid temperature data. Temperature data for the fine grid was available and used for SuperCOAST CAMx version 2 runs. Previous COAST CAMx version 1.13 model runs could not use this fine grid temperature data.

4. PERFORMANCE

After the execution of CAMx version for the SuperCOAST domain, model output was examined for reasonableness using PAVE and model performance statistics calculated. The statistics for the 1993 base case were calculated for the Houston-Galveston, Beaumont-Port Arthur and domain-wide area (Appendix B). Overall, model performance only changed slightly when compared to the 1993 base case for the COAST domain.

APPENDIX A: CAM$_x$ SuperCOAST Script

```
#
set TXDATA = "/stella/data/tnrcc/pgm/"
set EIDATA = "/stella/data/tnrcc/emis/"
set OUTDATA = "/stella/scratch/sarav/tnrcc/pgm"
set EP     = "0905"
set CASE   = "aak93"
set EMCASE   = "93babb"
set ELCASE   = "93b"
set ICBCCASE = "93basAj"
set COMCASE  = "93basAj"
set METCASE  = "93basAj"
set TESTER   = vukovich@ncsc.org
set WINDCASE = "super2"
set SCENBC = "uamv124_reg"

set INICBC   = "$TXDATA/$EP/$ICBCCASE/input/bc-ic-tc"
set INTC     = "$TXDATA/$EP/$ICBCCASE/input/bc-ic-tc"
set INCOMMON = "$TXDATA/$EP/$COMCASE/input/common"
set INLOEI   = "$EIDATA/$EP/$EMCASE"
set INELEI   = "$EIDATA/$EP/$ELCASE"
set INMET    = "$TXDATA/$EP/$METCASE/input/met"
set INWIND   = "$TXDATA/$EP/$WINDCASE/input/met"
set OUTPUT   = "$OUTDATA/$EP/$CASE/output"
set BINDIR   = "/env/proj/tnrcc/pgm/src/camx2.03"
#
date
#
if (-e CAMx.in) then
   /sbin/rm CAMx.in
endif
#
#   Script to Run CAMx
#
#  --- Create the day 1 input file (always called CAMx.in)
#
#
cat << ieof > CAMx.in
CAMx TCAS $CASE : one 16km grid, 930905 V2.03 (MCNC)
Root output name   |$OUTPUT/camx2.930905.$CASE
Start time/date    |1993 09 05    0.
End time/date      |1993 09 05 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 |23
                   |NO        NO2       O3        OLE       PAN       NXOY
                   |PAR       TOL       XYL       FORM      ALD2      ETH
                   |CRES      MGLY      OPEN      PNA       CO        HONO
                   |H2O2      HNO3      ISOP      MEOH      ETOH
Num fine nest      |0
SMOLAR or BOTT?    |SMOLAR
Restart            |false
Chemistry          |true
Dry dep            |true
Wet dep            |false
PiG submodel       |true
Staggered winds    |false
Treat area emiss   |true
```

```
Treat point emiss  |true
1-day emiss inputs |true
3-D average file   |true
Source Apportion   |false
Chemparam          |$INCOMMON/CAMx2.chemparm.3
Photolysis rates   |$INCOMMON/camx_photorate.930906-930911.isop.tcas_16km+hgbpa_04km.better
Landuse            |$INCOMMON/uamv_landuse.super_16km
Height/pressure    |$INMET/uamv_zp.930905.tcas_16km
Wind               |$INMET/uamv_wind.930905.tcas_16km.CAMx2
Temperature        |$INMET/uamv_temp.930905.tcas_16km.CAMx2
Water vapor        |$INMET/uamv_h2o.930905.tcas_16km
Cloud cover        |
Rainfall           |
Vertical diffsvty  |$INMET/uamv_kv.930905.tcas_16km
Initial conditions |$INICBC/uamv_ic.930905.clean
Boundary conditions|$INICBC/uamv_bc.930905
Top concentration  |$INTC/uamv_tc.clean
Albedo/haze/ozone  |$INCOMMON/uamv_aho.930905-930911.tcas_16km.tnrcc
Point emiss        |$INELEI/uamv_el_ei.930905.base
Area emiss         |$INLOEI/uamv_lo_ei.930905.base
Landuse         #1 |
Height/pressure #1 |
Wind            #1 |
Temperature     #1 |
Vertical diff   #1 |
Area emiss      #1 |
Coarse grid restart|
Fine grid restart  |
PiG restart        |
ieof
#
#  --- Execute the model ---
#
#/bin/time $BINDIR/CAMx |& tee $OUTPUT/camx2.930905.$CASE.out
#date
#
#Mail -s "930905 for $CASE completed" $TESTER <<-EOF
#The CAMx2 simulation for day = 930905
#has been completed.
#-EOF

#cp CAMx.in camx2.930905.$CASE.in
#

if (-e CAMx.in) then
   /sbin/rm CAMx.in
endif
#

cat << ieof > CAMx.in
CAMx SuperCOAST $CASE : one HG/BPA 4x4km subgrid, 930906 V2.03 (MCNC)
Root output name   |$OUTPUT/camx2.930906.$CASE
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 |23
                   |NO        NO2       O3        OLE       PAN       NXOY
                   |PAR       TOL       XYL       FORM      ALD2      ETH
                   |CRES      MGLY      OPEN      PNA       CO        HONO
                   |H2O2      HNO3      ISOP      MEOH      ETOH
Num fine nest      |1
```

```
net grid params    |31 50 23 37  8  4
SMOLAR or BOTT?    |SMOLAR
Restart            |false
Chemistry          |true
Dry dep            |true
Wet dep            |false
PiG submodel       |true
Staggered winds    |false
Treat area emiss   |true
Treat point emiss  |true
1-day emiss inputs |true
3-D average file   |true
Source Apportion   |false
Chemparam          |$INCOMMON/CAMx2.chemparm.3
Photolysis rates   |$INCOMMON/camx_photorate.930906-930911.isop.tcas_16km+hgbpa_04km.better
Landuse            |$INCOMMON/uamv_landuse.super_16km
Height/pressure    |$INMET/uamv_zp.930906.tcas_16km
Wind               |$INWIND/uamv_wind.930906.super_16km.CAMx2
Temperature        |$INMET/uamv_temp.930906.super_16km.CAMx2
Water vapor        |$INMET/uamv_h2o.930906.super_16km
Cloud cover        |
Rainfall           |
Vertical diffsvty  |$INMET/uamv_kv.930906.super_16km
Initial conditions |$INCOMMON/camx2.930905.$COMCASE.ic.bin
Boundary conditions|$INICBC/uamv_bc.930906
Top concentration  |$INTC/uamv_tc.clean
Albedo/haze/ozone  |$INCOMMON/uamv_aho.930906-930911.tcas_16km+hgbpa_04km
Point emiss        |$INELEI/egts.allpts.19930906.$ELCASE.super.bin
Area emiss         |$INLOEI/low_ei.super16km.19930906.$EMCASE.bin
Landuse         #1 |$INCOMMON/uamv_landuse.hgbpa_04km
Height/pressure #1 |$INMET/uamv_zp.930906.hgbpa_04km
Wind            #1 |$INMET/uamv_wind.930906.hgbpa_04km.CAMx2
Temperature     #1 |$INMET/uamv_temp.930906.hgbpa_04km.CAMx2
Vertical diff   #1 |$INMET/uamv_kv.930906.hgbpa_04km
Area emiss      #1 |$INLOEI/low_ei.4km.19930906.$EMCASE.bin
Coarse grid restart|
Fine grid restart  |
PiG restart        |
ieof
#
#  --- Execute the model ---
#
#/bin/time $BINDIR/CAMx |& tee $OUTPUT/camx2.930906.$CASE.out
date

#cp CAMx.in camx2.930906.$CASE.in

#Mail -s "930906 for $CASE completed" $TESTER <<-EOF
#The CAMx2 simulation for day = 930906
#has been completed.
#-EOF


foreach today ( 07 08 09 10 11 )
set yesterday = `echo $today | awk '{printf("%2.2d",$1-1)}'`
date
#
#
if (-e CAMx.in) then
   /sbin/rm CAMx.in
endif
#
#   Script to Run CAMx
#
#  --- Create the input file (always called CAMx.in)
#
```

```
cat << ieof > CAMx.in
CAMx TCAS $CASE : one HG/BPA 4x4km subgrid, 9309$today V2.00 (MCNC)
Root output name   |$OUTPUT/camx2.9309$today.$CASE
Start time/date    |1993 09 $today    0.
End time/date      |1993 09 $today 2400.
DT:max,in,emis,out |0.5 1. 1. 1.
nx,ny,nz           |95  83  8
Coordinate ID      |UTM
xorg,yorg,dx,dy,uzn|-316. 2808.  16.  16.  15
time zone          |6
PiG parameters     |2000. 12.
Avg output species |23
                   |NO        NO2       O3        OLE       PAN       NXOY
                   |PAR       TOL       XYL       FORM      ALD2      ETH
                   |CRES      MGLY      OPEN      PNA       CO        HONO
                   |H2O2      HNO3      ISOP      MEOH      ETOH
Num fine nest      |1
net grid params    |31 50 23 37  8  4
SMOLAR or BOTT?    |SMOLAR
Restart            |true
Chemistry          |true
Dry dep            |true
Wet dep            |false
PiG submodel       |true
Staggered winds    |false
Treat area emiss   |true
Treat point emiss  |true
1-day emiss inputs |true
3-D average file   |true
Source Apportion   |false
Chemparam          |$INCOMMON/CAMx2.chemparm.3
Photolysis rates   |$INCOMMON/camx_photorate.930906-930911.isop.tcas_16km+hgbpa_04km.better
Landuse            |$INCOMMON/uamv_landuse.super_16km
Height/pressure    |$INMET/uamv_zp.9309$today.tcas_16km
Wind               |$INWIND/uamv_wind.9309$today.super_16km.CAMx2
Temperature        |$INMET/uamv_temp.9309$today.super_16km.CAMx2
Water vapor        |$INMET/uamv_h2o.9309$today.super_16km
Cloud cover        |
Rainfall           |
Vertical diffsvty  |$INMET/uamv_kv.9309$today.super_16km
Initial conditions |
Boundary conditions|$INICBC/uamv_bc.9309$today
Top concentration  |$INTC/uamv_tc.clean
Albedo/haze/ozone  |$INCOMMON/uamv_aho.930906-930911.tcas_16km+hgbpa_04km
Point emiss        |$INELEI/egts.allpts.199309$today.$ELCASE.super.bin
Area emiss         |$INLOEI/low_ei.super16km.199309$today.$EMCASE.bin
Landuse         #1 |$INCOMMON/uamv_landuse.hgbpa_04km
Height/pressure #1 |$INMET/uamv_zp.9309$today.hgbpa_04km
Wind            #1 |$INMET/uamv_wind.9309$today.hgbpa_04km.CAMx2
Temperature     #1 |$INMET/uamv_temp.9309$today.hgbpa_04km.CAMx2
Vertical diff   #1 |$INMET/uamv_kv.9309$today.hgbpa_04km
Area emiss      #1 |$INLOEI/low_ei.4km.199309$today.$EMCASE.bin
Coarse grid restart|$OUTPUT/camx2.9309$yesterday.$CASE.inst.2
Fine grid restart  |$OUTPUT/camx2.9309$yesterday.$CASE.finst.2
PiG restart        |$OUTPUT/camx2.9309$yesterday.$CASE.pig
ieof
#
#  --- Execute the model ---
#
/bin/time $BINDIR/CAMx  |& tee $OUTPUT/camx2.9309$today.$CASE.out
date
#
Mail -s "9309$today for $CASE completed" $TESTER <<-EOF
The CAMx2 simulation for day = 9309$today
has been completed.
-EOF
```

```
#
cp CAMx.in camx2.9309$today.$CASE.in
#
end
Mail -s "CAMx2 run for $CASE Complete" $TESTER << -EOF
The CAMx2 simulation for $CASE has been completed.
-EOF

date

exit
```

APPENDIX B: PERFORMANCE STATISTICS

4.0.1 SuperCOAST

```
MODEL PERFORMANCE INDICATORS:
RUN ID: SUPER COAST CAMx 93basAj - 9/08/93


O3        : Between the Hours of  1. and 24. on  93251

                         OBSERVED VALUE GREATER THAN 60.00  ppb            OBSERVED VALUE > 0.0 ppb

                         --------------------------------------------      ------------------------
Number of Data Pairs:                371                                              798

Max Domain-wide Sim Value :      188.059  ppb

Max Station-wide Sim Value:      177.825  ppb                                     177.825  ppb

Maximum Observed Value:          214.000  ppb                                     214.000  ppb

Domain-wide Unpaired Acc.:        -0.121

Station-wide Unpaired Acc.:       -0.169

Average Accuracy of Peak:          0.027                                             0.027

Normalized Bias :                  0.018

Normalized Gross Error:            0.213

Fractional Bias :                 -0.019

Fractional Gross Error:            0.215

Ratio of Bias to Mean Obs:        -0.004                                             0.081

Ratio Gross Error to Mean Obs:     0.212                                             0.349

Maximum Residual:                 74.377  ppb                                      74.377  ppb

Minimum Residual:                -81.728  ppb                                     -81.728  ppb

Mean Unsigned Error:              19.455  ppb                                      19.783  ppb

Mean residual:                    -0.325  ppb                                       4.586  ppb

Mean Simulated Value:             91.365  ppb                                      61.321  ppb

Mean Observation:                 91.690  ppb                                      56.736  ppb

Root Mean Sqare Error:            25.360  ppb                                      25.149  ppb
```

```
Std. Deviation of Fract Bias:      0.282
*****************************************************************************************************


MODEL PERFORMANCE INDICATORS:
RUN ID: SUPER COAST CAMx 93basAj - 9/09/93

O3        : Between the Hours of  1. and 24. on  93252

                         OBSERVED VALUE GREATER THAN 60.00  ppb             OBSERVED VALUE > 0.0 ppb

                         ---------------------------------------------       ------------------------
Number of Data Pairs:                336                                                   811

Max Domain-wide Sim Value :      173.107  ppb

Max Station-wide Sim Value:      163.855  ppb                                         163.855  ppb

Maximum Observed Value:          195.000  ppb                                         195.000  ppb

Domain-wide Unpaired Acc.:        -0.112

Station-wide Unpaired Acc.:       -0.160

Average Accuracy of Peak:          0.081                                                0.106

Normalized Bias :                 -0.002

Normalized Gross Error:            0.228

Fractional Bias :                 -0.054

Fractional Gross Error:            0.243

Ratio of Bias to Mean Obs:        -0.027                                                0.082

Ratio Gross Error to Mean Obs:     0.225                                                0.379

Maximum Residual:                 63.633  ppb                                          87.818  ppb

Minimum Residual:                -94.765  ppb                                         -94.765  ppb

Mean Unsigned Error:              19.489  ppb                                          20.901  ppb

Mean residual:                    -2.325  ppb                                           4.540  ppb

Mean Simulated Value:             84.425  ppb                                          59.728  ppb

Mean Observation:                 86.750  ppb                                          55.189  ppb

Root Mean Sqare Error:            26.172  ppb                                          27.351  ppb

Std. Deviation of Fract Bias:      0.355
*****************************************************************************************************

MODEL PERFORMANCE INDICATORS:
RUN ID: SUPER COAST CAMx 93basAj - 9/10/93
```

```
O3        : Between the Hours of  1. and 24. on  93253

                         OBSERVED VALUE GREATER THAN 60.00  ppb           OBSERVED VALUE > 0.0 ppb
                         -------------------------------------------      -------------------------
Number of Data Pairs:                397                                                   834

Max Domain-wide Sim Value :      177.782  ppb

Max Station-wide Sim Value:      168.834  ppb                                         168.834  ppb

Maximum Observed Value:          162.000  ppb                                         162.000  ppb

Domain-wide Unpaired Acc.:         0.097

Station-wide Unpaired Acc.:        0.042

Average Accuracy of Peak:         -0.052                                                -0.028

Normalized Bias :                 -0.096

Normalized Gross Error:            0.235

Fractional Bias :                 -0.160

Fractional Gross Error:            0.282

Ratio of Bias to Mean Obs:        -0.113                                                -0.003

Ratio Gross Error to Mean Obs:     0.238                                                 0.348

Maximum Residual:                 43.146  ppb                                          52.777  ppb

Minimum Residual:                -97.540  ppb                                         -97.540  ppb

Mean Unsigned Error:              21.520  ppb                                          20.173  ppb

Mean residual:                   -10.233  ppb                                          -0.166  ppb

Mean Simulated Value:             80.293  ppb                                          57.881  ppb

Mean Observation:                 90.526  ppb                                          58.047  ppb

Root Mean Sqare Error:            29.482  ppb                                          26.564  ppb

Std. Deviation of Fract Bias:      0.390
*****************************************************************************************************
MODEL PERFORMANCE INDICATORS:
RUN ID: SUPER COAST CAMx 93basAj - 9/11/93

O3        : Between the Hours of  1. and 24. on  93254

                         OBSERVED VALUE GREATER THAN 60.00  ppb          OBSERVED VALUE > 0.0 ppb
                         -------------------------------------------     -------------------------
Number of Data Pairs:                284                                                   848

Max Domain-wide Sim Value :      185.906  ppb
```

Max Station-wide Sim Value:	132.303	ppb	132.303	ppb
Maximum Observed Value:	189.000	ppb	189.000	ppb
Domain-wide Unpaired Acc.:	-0.016			
Station-wide Unpaired Acc.:	-0.300			
Average Accuracy of Peak:	-0.063		-0.016	
Normalized Bias :	0.007			
Normalized Gross Error:	0.179			
Fractional Bias :	-0.024			
Fractional Gross Error:	0.183			
Ratio of Bias to Mean Obs:	-0.025		0.096	
Ratio Gross Error to Mean Obs:	0.179		0.360	
Maximum Residual:	55.051	ppb	66.404	ppb
Minimum Residual:	-106.087	ppb	-106.087	ppb
Mean Unsigned Error:	15.794	ppb	16.626	ppb
Mean residual:	-2.169	ppb	4.422	ppb
Mean Simulated Value:	85.839	ppb	50.640	ppb
Mean Observation:	88.007	ppb	46.218	ppb
Root Mean Sqare Error:	23.051	ppb	22.099	ppb
Std. Deviation of Fract Bias:	0.259			

****