

## 7.4 HIGH-RESOLUTION REAL-TIME OZONE FORECASTS FOR THE AUGUST-SEPTEMBER TEXAS AQS-2000 (HOUSTON) FIELD STUDY: FORECAST PROCESS AND PRELIMINARY EVALUATION

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### 1. INTRODUCTION\*

For the last several years, we have reported on the implementation and production of atmospheric chemical forecasts using a real-time numerical air quality prediction (NAQP) system (McHenry, et al., 2000; McHenry et al., 1999). The system that we have developed makes use of a tripartite set of models implemented on parallel micro-processor scalar computers in real-time. These models include the Penn. State/NCAR MM5 (Grell et al., 1994), Version 2.12; the Sparse-Matrix Operator Kernel Emissions (SMOKE, Coats et al., 1996) processing/modeling system, and a real-time version of the Multiscale Air Quality Simulation Platform photochemical grid model (MAQSIP-RT, Odman and Ingram, 1996; Srivastava et al., 1994), closely related to EPA's Models-3/CMAQ (EPA, 1999).

By applying the modeling system quasi-continuously for three summers, we have been able to archive model outputs for later evaluation on a wider variety of cases than is normally accomplished through study of selected, poor-air-quality scenarios alone. This "discipline of forecasting" has been cited in a report by the National Research Council's Board on Atmospheric Sciences and Climate (BASC: Entering the 21<sup>st</sup> Century, 1998) as a *necessary next step* for continuing to advance the state of the atmospheric-environmental sciences as we enter the new millennium.

As a partial result of this process, MAQSIP has been shown to have measurable forecast skill in the northeast US deployed as a regional, 36km-scale model. Objectively, 17 of 19 forecasts evaluated had skill, with 10 of those 17 meeting four different skill criteria: (1) threat score > .20; (2)  $R^2 > .2$ ; (3) mean-absolute error < 15PPB vis-à-vis surface monitors reporting above 60PPB on "clean days" and above

80PPB on "dirty days;" and (4) absolute bias error < 7PPB.

Recently, the MM5/SMOKE/MAQSIP modeling system was also evaluated for a season-long (June 1 – August 31, 1995) retrospective application (Hogrefe et al., 2000a; Hogrefe et al., 2000b). In this study, MAQSIP ozone simulations were compared against observations and a second photochemical modeling system consisting of the RAMS3b (Walko et al., 1995) and UAM-V (SAI, 1995) models. Using spectral-scale analysis to decompose the model results and observations into characteristic time-scales (seasonal-background, synoptic, diurnal, and intra-day), it was shown that UAM-V underestimates the total variance of the ozone time series (energy) when compared with the observations, but shows a higher mean value than the observations.

On the other hand, *MAQSIP was better able to reproduce the average energy and mean concentration of the observations*. However, neither modeling system was able to capture the sub-diurnal variability, primarily due to the relatively coarse resolution of the 36km grid-spacing.

As pointed out by Rao et al. 1997, the level of spacing in an observational monitoring system needed to capture all of the 1-hour, 120PPB ozone exceedances that actually occur in nature would be about 5km. Thus, we expect that a 5km grid-spacing for a photochemical model would be an upper limit on the model grid-spacing required to resolve all of the fine-scale variability, including the full signal amplitude, contained in the monitor data.

Given these encouraging results for both retrospective and real-time forecast simulations at 36km grid-spacing, the summer of 2000 presented a timely opportunity to apply and evaluate MAQSIP-RT at a much higher, 5km grid-resolution. These forecasts were accomplished as part of the numerical support for the large, multi-institution Texas Air Quality Study-2000 (TXAQS-2000) field program conducted in Houston, Texas from August 15 through September 15, 2000. In this field program, four aircraft and many additional/special ground-based measurement

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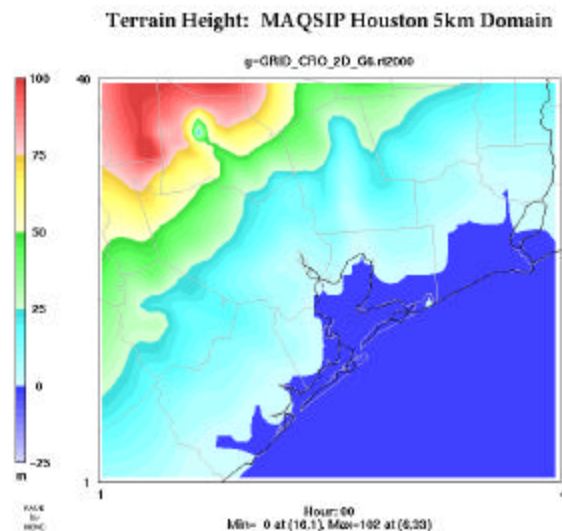
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systems were utilized in order to attempt a relatively complete 3-dimensional observational characterization of the meteorology and atmospheric chemistry of the Houston metropolplex, one of the two most polluted metropolitan locales in the U.S. The modeling system as deployed for TXAQS-2000 is known as the Real-time Ozone Forecast System-2000, or RTOFS-2000.

In this paper, we review the RTOFS-2000 component models, model coupling, and model initialization for TXAQS-2000. We then discuss the forecast process as the modeling system was used during the field program. Next, we summarize the metrics and data being used in the preliminary performance analysis. Because the actual analysis was still incomplete at the time of abstract submittal, the results of the analysis will be presented at the conference. We conclude with a brief summary and an outlook for the future.

## 2. COMPONENT MODELS

MM5 has been run in real-time at the North Carolina Supercomputing Center for the past two years. Twice-daily, initial and boundary conditions are constructed after downloading 40km Lambert-conformal, Grid-212 Eta-model GRIB forecast files from the National Centers for Environmental Prediction (NCEP). MM5's coarse (45km) domain covers much of North America from the central Canada south to the Yucatan Peninsula, and includes portions of the eastern Pacific and western Atlantic. The fine 15km domain covers the Eastern two-thirds of the United States, and the very high-resolution (VHR) domain is about 200km on a side centered on Houston, Texas. All MM5 domains use a Lambert conformal map projection with 31 sigma-coordinate layers in the vertical. Model top is fixed at 100mb. The MAQSIP-RT domains are windows into these MM5 domains and share this common vertical structure. The MAQSIP-RT TXAQS-2000 Houston domain is shown in Figure 1. Refer to <http://envpro.ncsc.org/projects/SECMEP/secmep.html> for more details.



**Figure 1. MAQSIP TXAQS-2000 5km-grid-spacing domain showing terrain height (meters). Galveston Bay is at center; metro Houston is just northwest of Galveston Bay.**

MM5 is configured with a high-resolution planetary boundary layer scheme ( Zhang and Anthes, 1982), a deep convection scheme (Kain and Fritsch, 1993), a simple ice phase explicit moisture scheme, an atmospheric radiation scheme (Dudhia, 1989), and a five-layer soil heat-diffusion model with climatological moisture availability.

MAQSIP-RT is a highly optimized version of MAQSIP that uses a modified version of the Carbon Bond IV (Gery et al., 1989) chemical mechanism, a flux-form advection scheme (Bott, 1989), a K-theory scheme for turbulent vertical re-distribution of pollutants (Alapaty et al., 1997), and a dry deposition scheme (Walcek, et al., 1986). Clear-sky photolysis rates are calculated following Madronich (1987). It also uses an innovative cloud processes package which represents the effects of deep and shallow convection, grid-scale stratiform/cirruform layer clouds, and additional sub-grid scale layer clouds. Both the cloud package and turbulence parameterization were discussed in McHenry et al., 1999. A top-boundary condition has been added based on lower stratospheric monthly mean ozone data (Logan, 1999).

SMOKE is a high-efficiency emissions-processing system. It features several hundred-fold computational performance enhancements due to its sparse-matrix algorithms for factor-based computations. The RTOFS-2000 simulations used SMOKE to process a composite inventory that was assembled from "best available" components. The Ozone Transport Assessment Group (OTAG) 1995 inventory (Pechan,

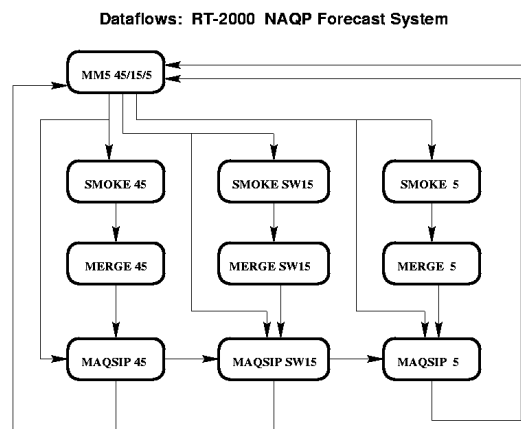
1995) was used for offshore point sources; the NET-V3.11 1996 inventory (EPA, 2000) was used for point sources outside Texas and for area and non-road sources; the TNRCC "DFW" 1996 inventory was used for point sources within Texas; the SMRAQ 1995 (Houyoux et al., 2000) inventory was used for mobile source emissions; and the Biogenic Emissions Landcover Dataset 3 (BELD3, Pierce et al., 1998) was used for biogenic sources. For RTOFS-2000, no attempt was made to project these generally mid-1990's inventories to the year 2000.

RTOFS-2000 used real-time *forecast* meteorology to supply SMOKE with data needed to model meteorologically sensitive emissions such as biogenic and vehicular emissions, and point-source plume rise. Because of the higher vertical resolution in third-generation models, SMOKE's discretization of plume rise *for every point source* was used.

### 3. MODEL COUPLING

Figure 2 shows the high-level dataflow diagram for RTOFS-2000. The MCPL output module (Coats et al., 1998) is used within MM5 to generate outputs compatible with SMOKE and MAQSIP, which both use an I/O Applications Programming Interface (I/O API, Coats, 1995). The present I/O API implementation is layered on top of NetCDF from the National Center for Atmospheric Research and PVM from Oak Ridge National Laboratory, although the I/O API was designed from the beginning so that this lower layer could be easily changed.

MCPL fits into MM5 with minimal effort, and is callable at a variety of time scales from the advection-step frequency on up. It provides functionality generalizing the present MM5 subroutine "OUTTAP." MCPL is extremely flexible and configurable, allowing selected output variables, output formats, and windows into MM5 nests, all through the use of environment variable flags.



**Figure 2. High Level data flow diagram for RTOFS-2000.**

As Figure 2 indicates, MM5 (top left) is run on all three domains simultaneously. The coarse-most, 45km domain produces a 60-hour forecast, whereas the 15km domain produces a 24-hour forecast spawned at 21z when the 12z cycle is running, and at 08z when the 00z forecast is running. The 5km Houston VHR domain is spawned from the 08z 15km domain at 11z, allowing for a complete daytime simulation before shutting off at 23z.

These MM5 domains each provide data to domain-specific instantiations of SMOKE, which processes the components of the composite inventory separately but in parallel. These components are then merged in a final step on all 3 domains before the complete inventory is provided to MAQSIP-RT. Each SMOKE instantiation and the 45km MAQSIP-RT all run in parallel with MM5. Following the completion of this group of parallel runs, the 15km and 5km MAQSIP-RTs run in parallel, with the 15km MAQSIP-RT providing time-dependent boundary conditions to the 5km Houston VHR MAQSIP-RT.

Because MAQSIP-RT is highly optimized, the 00z-cycle forecasts completed in time for post-processing and delivery of VIS5D files and Web-based products to TNRCC and the forecast and flight operations groups at TXAQS-2000, meeting a 7AM CDT schedule deadline. For the 12z cycle, no 5km simulation was required.

### 4. MODEL INITIALIZATION

There is little *real-time* atmospheric chemical measurement data suitable for use in initializing an NAQP model. Real-time ground-level primary precursor data (NO<sub>x</sub>, VOC) are collected, but assembly for use in real-time presents geopolitical and database



For boundary conditions, clean tropospheric background concentrations are set on the boundaries of the coarse domain for all atmospheric trace species except ozone. For ozone, a monthly varying mean observed ozone profile has been employed above 500mb (Logan, 1999). The 15km-scale and VHR domains utilize time-dependent chemical boundary conditions provided by the coarse domain(s) MAQSIP-RT run.

## 5. FORECAST PROCESS

During TXAQS-2000, weather and ozone outlook briefings were provided to the experimentalists and flight operations groups responsible for aircraft deployment and data collection. To conduct the briefings, a forecast team was assembled by Professor John Neilson-Gammon at Texas A&M University consisting of himself and two assistants.

There was an “all-hands” briefing conducted at 7AM CDT in the main meeting room of the project headquarters occupying temporary office space at Ellington Field just southeast of downtown Houston. An update to the 7AM briefing was provided at 1PM and included outlooks for tomorrow and the next day. The briefings featured observations, objective model guidance, and subjective interpretations. Most of the observations and objective model guidance was collected on a project forecast Website located at: (<http://www.met.tamu.edu/t2k>). These tools consisted of high-resolution satellite imagery processed at TNRCC, Texas A&M, and NASA,; meteorological model output including MCNC’s MM5, Texas A&M’s MM5, and the NCEP model suite; chemical model guidance including MAQSIP-RT, an integrated meteorological-chemical forecast model run at NOAA’s Forecast Systems Lab (FSL), and the HYSPLIT model run at NOAA’s Air Resources Lab; raw alphanumeric data including METAR format data; radar data; near-Houston surface observations of ozone provided by TNRCC; buoy data from the Texas Automated Buoy system and from the Houston-Galveston PORTS system; profiler data; and radiosounding data.

MAQSIP-RT data was provided to the forecast team in two forms: (1) a Website with a java-script-enabled animator containing the following products: forecast ozone on all 3 model domains for the lowest model layer (about 18m AGL) and 8 layers aloft including 5 layers within the daytime PBL; lowest layer forecast  $H_2O_2$ ,  $HNO_3$ ,  $NO_x$ , PAN, and Isoprene; accumulated nitrate (and ozone, though very small) wet deposition; and cloud properties such as fractional coverage, cloud type, and below cloud clear-sky “J” multiplier due to cloud attenuation of actinic flux; and (2) VIS5D files on all three domains containing the

following 3D forecast fields: ambient temperature, cloud-water mixing ratio, U, V, and W wind components, NO,  $NO_2$ ,  $O_3$ ,  $H_2O_2$ , CO, formaldehyde, and isoprene.

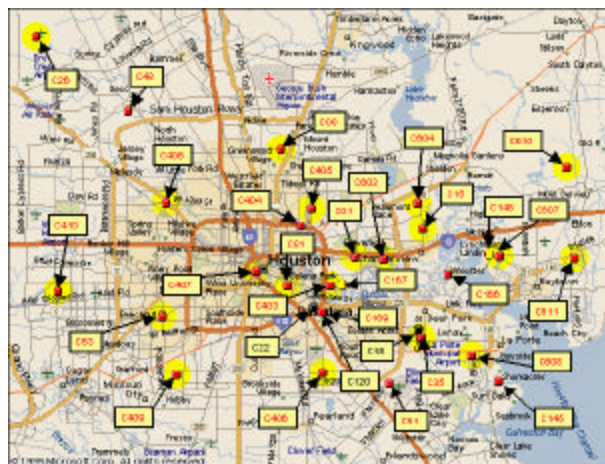
The Web-based products were generally used during the “all-hands” briefings as part of the larger forecast process, which also included many of the tools mentioned above on a day-in-day-out basis. The VIS5D products were used on a computer in a separate office for individual analysis and interpretation by the forecasters.

## 6. PRELIMINARY MAQSIP-RT FORECAST PERFORMANCE

A reasonably thorough statistical evaluation of the MAQSIP-RT VHR Houston surface-layer ozone forecasts conducted for TXAQS-2000 is being performed.



**Figure 4. A Subset of Houston metroplex surface ozone monitor sites being used for MAQSIP-RT evaluation.**



**Figure 5. Monitor locations providing surface ozone data near downtown Houston (inset from Figure 4.)**

To do this, MAQSIP-RT forecasts are being evaluated against data obtained from 48 surface ozone monitor sites in and around metro-Houston. A map showing some of the sites is presented in Figures 4 and 5.

During TXAQS-2000, a total of 18 VHR 12-hour forecasts were delivered, beginning on Aug 26<sup>th</sup> and ending on Sept. 15<sup>th</sup>. An additional nine forecasts, from Sept 16<sup>th</sup> through Sept 25<sup>th</sup> (with the exception of the 23<sup>rd</sup>) were completed and are participating in the evaluation, for a total of 27 forecasts. Though TXAQS-2000 began on Aug. 15<sup>th</sup>, aircraft operations did not begin until the week of the 22<sup>nd</sup>. Thus, despite minor RTOFS-2000 implementation delays, the forecasts were well-coordinated with the actual flight operations.

The statistical measures that are being used are quite standard and include both time-series and contour overlays of MAQSIP-RT forecast ozone versus observations. For each monitor, the following time series are being produced:

- Day-by-day monitor versus model forecasts (one value per day for 27 days), showing the entire period trend, for the following: daily maximum ozone, daily minimum ozone, and daily mean ozone.
- Day-by-day differences of monitor--model forecasts for the following: daily mean difference and daily RMS difference.
- Hourly monitor versus model forecasts for each forecast day, including: hourly mean observation, MAQSIP-RT hourly mean, hourly maximum, and hourly minimum.

In addition, aggregated over all 48 monitor sites in the entire domain, for each date, the following time series are being computed:

- Hourly values for each forecast day, including: observed maximum, minimum, and mean ozone plotted against MAQSIP-RT forecast maximum, minimum, and mean ozone.
- Hourly differences of monitor—model forecasts for the following: minimum difference, maximum difference, mean difference, and RMS difference.

Finally, aggregated over all 48 monitors and averaged daily, we produce the following time series:

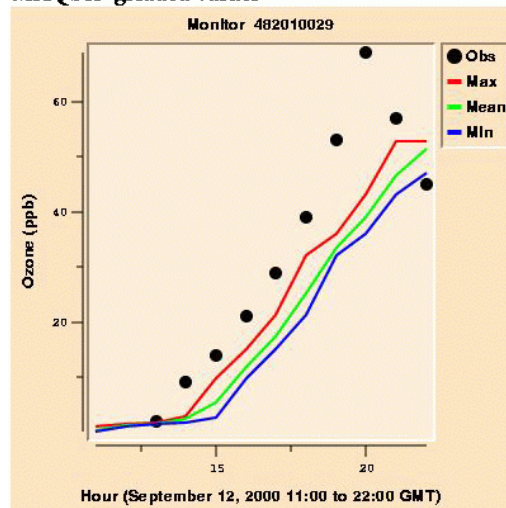
- Day-by-day (one value per day for 27 days) mean and RMS monitor—model difference.

All of the above metrics, along with the contour overlays, are being provided on the analysis Webpage shared between MCNC and TNRCC. Though not as rigorous as the analysis conducted by Hogrefe et al., 2000b, this approach will allow us to make fairly reliable inferences about both the mean spatial-temporal behavior of the forecast model and the high-frequency behavior in the intra-day period. We would expect that at the VHR resolution used, the model would exhibit a wider range of forecast ozone values than it does at the much coarser-scales studied in the above referenced work. The metrics will also allow us to look at features such as phase delays – whereby the model might have forecast the ozone maxima correctly but displaced its formation, a result that could stem from either meteorological or chemical factors.

For the purposes of illustration, we provide example plots for intra-day hourly monitor—model time series for four of the monitor locations shown in Figures 4 and 5 for Sept 12, the only day for which comparisons had been generated at press time. These four locations are chosen as representative of the Houston metroplex and are circled in Figures 4 and 5. The first is in northwest Harris County (CAMS26 – Figure 6), the second in Galveston (CAMS34 – Figure 7), the third in central downtown Houston (CAMS81 – Figure 8) and the fourth near the ship channel at LaPorte (CAMS608 – Figure 9).

Grid: 05km Houston metropolitan area (g6)  
Date: Tue Sep 12 2000 (20000912)  
Monitor: Northwest Harris Co. C26/C110/C154 (482010029)

**MAQSIP gridded values**



**Figure 6. MAQSIP-RT time-series versus observations at Northwest Harris County for Sept. 12, 2000**

Northwest Harris county often experiences elevated ozone amounts during events in which the wind is directed toward the northwest from downtown Houston. Though this particular day was relatively clean, it can be seen (Figure 6) that both model and observations peak late in the day, around 20z. At this monitor, and also with the downtown Houston (Figure 8) and near-ship-channel monitors (Figure 9), the agreement is quite good, admitting a slight under-forecast compared to the observed peaks. A slight phase lag (MAQSIP-RT peaks slightly later than the observations) at LaPorte is also in evidence.

At Galveston, the forecast is fairly well correlated with the observations but biased low. Evidently there was a modest ozone plume that advected across the Galveston monitor that was not well-simulated by the model.

In general, these plots and others suggest that MAQSIP-RT does have the potential to exhibit forecast skill at this VHR scale. The variability in the model simulation appears to be tracking fairly well with the observations, suggesting that more of the intra-day signal is being resolved than in the more coarse-scale version of the model studied in Hogrefe et al. (2000b). It should be cautioned, however, that this was an arbitrarily chosen day that turned out to be clean and cannot be extrapolated to other days in the evaluation period.

Grid: 05km Houston metropolitan area (g6)  
 Date: Tue Sep 12 2000 (20000912)  
 Monitor: Galveston Airport C34/C109/C152 (481670014)

**MAQSIP gridded values**

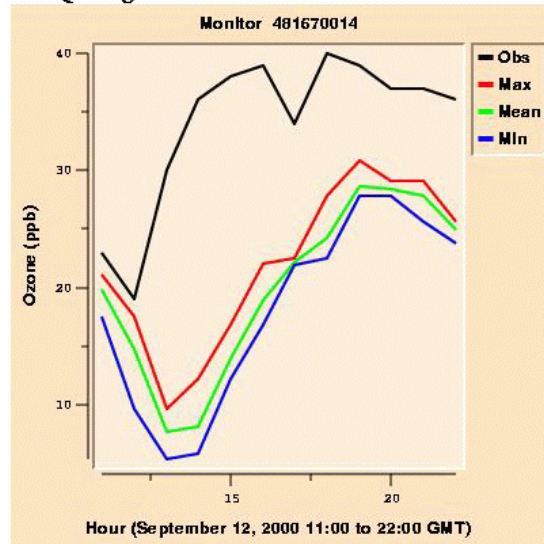


Figure 7. MAQSIP-RT time-series versus observations at Galveston for Sept. 12, 2000

We will present a more comprehensive picture of the entire evaluation at the conference.

## 7. DISCUSSION AND CONCLUSIONS

In this paper we have described the implementation and delivery of very-high resolution real-time forecasts in support of the Texas Air Quality Study-2000. We have described the history of the NAQP project at MCNC and the results of several previous evaluations of the MAQSIP model used in this study. We briefly reviewed the models involved, their coupling, and their dataflows as implemented in RTOFS-2000.

We discussed the model initialization procedure including a novel real-time data assimilation system, which ingests observed ozone data from over 900 monitors on a daily basis.

Finally, we provided an overview of the preliminary evaluation in progress, and provided some examples of model versus observed time series for monitors representative of the Houston metroplex.

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TNRCC views and no official endorsement should be inferred. Mention of trade names/products does not imply official endorsement.

Grid: 05km Houston metropolitan area (g6)  
 Date: Tue Sep 12 2000 (20000912)  
 Monitor: Houston Regional Office C81 (482010070)

**MAQSIP gridded values**

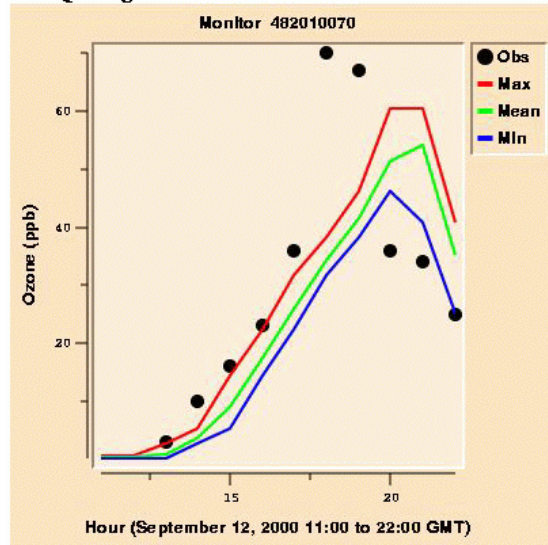


Figure 8. MAQSIP-RT time-series versus observations in downtown Houston for Sept. 12, 2000

Grid: 05km Houston metropolitan area (g6)  
 Date: Tue Sep 12 2000 (20000912)  
 Monitor: HRM-8 LaPorte C608 (482010808)

**MAQSIP gridded values**

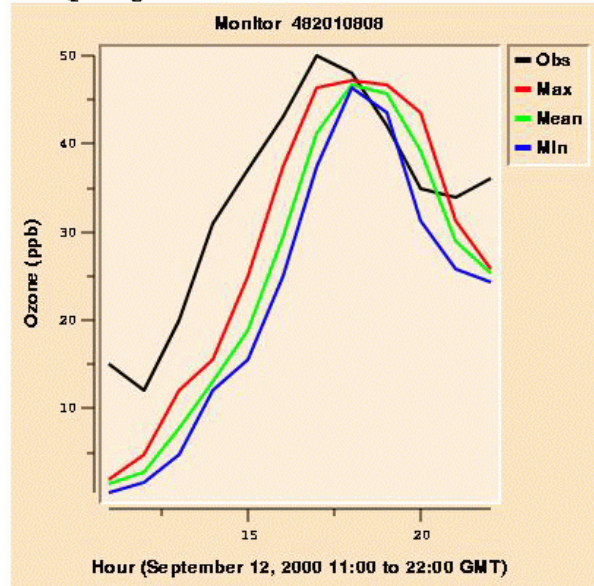


Figure 9. MAQSIP-RT time-series versus observations at LaPorte for Sept. 12, 2000

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