Semiannual Progress Report on the Project:

"Modeling the Transport and Chemical Evolution of Onshore and Offshore Emissions and Their Impact on Local and Regional Air Quality Using a Variable-Grid-Resolution Air Quality Model"

Type of Report:	Semiannual progress report
Reporting Period:	10/17/2003 - 04/16/2004
Principal Author:	Kiran Alapaty
Date Report was Issued:	May 17, 2004
DOE Award Number:	DE-FC26-03NT15466
Submitting Organization:	Carolina Environmental Program University of North Carolina at Chapel Hill Bank of America Plaza, CB# 6116 137 E. Franklin Street Chapel Hill, NC 27599-6116

Disclaimer

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

Abstract

This document, the project's second semiannual report, summarizes the research performed from 10/17/2003 through 04/16/2004, the second half of the first project year. Portions of the research in several of the project's eight tasks were completed, and the results obtained are briefly presented. We found that usage of a simpler boundary layer scheme compared to a sophisticated boundary layer scheme resulted in better simulation of mesoscale dynamical features, particularly when using high-resolution grids. Utilization of a new surface data assimilation technique has resulted in improved meteorological simulations across all domains using different resolution grids. Ingestion of remotely sensed sea surface temperatures into a high-resolution domain resulted in a marginal improvement in the model simulations. After evaluating all these results, we have finalized a best modeling configuration that leads to simulation of improved meteorological fields for use in variable-grid-resolution air quality simulation models. Development of the variable-grid-resolution emission modeling system is still in progress; we anticipate that it will be completed during the second project year. We have also completed development and testing of a cloud mixing algorithm for use in the variable-grid-resolution air quality simulation model.

Contents

Disclaimer ii

Abstract iii

Section 1: Experimental 1

1.1 Project Objectives 1

1.2 Task Descriptions 1

1.2.1 Task 1: Develop Modeling Domains and Case Studies 1

1.2.2 Task 2: Improve the Representation of Boundary Layer Processes 2

1.2.3 Task 3: Assimilation of Surface Observations to Improve MM5 Simulations 2

1.2.4 Task 4: Simulate Mesoscale Circulations Using the MM5 3

1.2.5 Task 5: Develop Emission Estimates 3

1.2.6 Task 6: Enhance Representation of Cloud Processes in the MAQSIP-VGR 3

1.2.7 Task 7: Perform Simulations and Evaluation of the MAQSIP-VGR over the Houston-Galveston Domain 4

1.2.8 Task 8: Perform Simulations and Evaluation of the MAQSIP-VGR over the Northeast Gulf Domain 4

Section 2: Results and Discussion 4

2.1 Develop Modeling Domains and Case Studies (Task 1) 4

2.2 Improve the Representation of Boundary Layer Processes (Task 2) 5

2.3 Assimilation of Surface Observations to Improve MM5 Simulations (Task 3) 16

2.3.1 Assimilation of Land-based Surface Observations using the FASDAS 16

2.3.2 Ingestion of Satellite-Measured Sea Surface Temperatures into the MM5 26

2.4 Simulate Mesoscale Circulations Using the MM5 (Task 4) 33

2.5 Develop Emission Estimates (Task 5) 33

2.5.1 Enhancing the SMOKE Configuration 33

2.5.2 Updating the Emissions Inventory 33

2.6 Enhance Representation of Cloud Processes in the MAQSIP-VGR (Task 6) 34

2.7 Perform Simulations and Evaluation of the MAQSIP-VGR over the Houston-Galveston Domain (Task 7) 34

2.8 Perform Simulations and Evaluation of the MAQSIP-VGR over the Northeast Gulf Domain (Task 8) 34

Section 3: Conclusion 35

Section 4: Publications 36

References 37

Section 1: Experimental

1.1 Project Objectives

This research project has two primary objectives:

(1) to further develop and refine the Multiscale Air Quality Simulation Platform – Variable Grid Resolution (MAQSIP-VGR) model, an advanced variable-grid-resolution air quality model, to provide detailed, accurate representation of the dynamical and chemical processes governing the fate of anthropogenic emissions in coastal environments; and

(2) to improve current understanding of the potential impact of onshore and offshore oil and gas exploration and production (E&P) emissions on O_3 and particulate matter nonattainment in the Gulf of Mexico and surrounding states.

1.2 Task Descriptions

There are eight tasks to be completed during the first two years of the project and two tasks for the final year. This first semiannual report provides detailed descriptions of research work performed during the first half of the project first year. The rest of this section provides brief descriptions of the first eight tasks. Section 2, "Results and Discussion," describes what has been completed in each of these tasks, Section 3 presents conclusions, and Section 4 presents a list of conference/workshop presentations and possible journal articles that may be developed during the course of this project.

1.2.1 Task 1: Develop Modeling Domains and Case Studies

The meteorological modeling domains will be configured with various horizontal grid resolutions. We propose to use grid resolutions of 36, 12, and 4 km. The 36-km resolution grid will cover a region extending west of the Atlantic Ocean westward to the Rockies; a grid at this coarse resolution will allow meteorological modeling simulations that are computationally inexpensive, and whose results will be used primarily to provide lateral boundary conditions to the nested grids. The 12-km grids will cover portions of Southern and Southeastern states. The 4-km grids will cover domains specific to addressing air pollution issues proposed in this study.

Selection of the time periods simulated for the case studies will be based on analysis of measurement data and the availability of offshore emissions activity data. The choice will also consider other current and prior modeling efforts (e.g., the Gulf Coast ozone study); simulating similar time periods will allow us to cross-compare and evaluate our modeling results against others available for the region.

The MAQSIP-VGR simulation domain will cover the Gulf of Mexico and some inland parts of surrounding states. Our air quality modeling analyses will focus on two geographical regions of

the Gulf Coast. The variable-grid mesh for these regions will consist of grid resolutions ranging from 400 m to 4 km, while the grid resolution for the areas beyond these two regions of interest will have grid resolutions ranging from 4 km to 12 km. The time-dependent lateral boundary conditions for this grid-mesh configuration will be obtained from regional uniform grid simulations of the MAQSIP-VGR.

1.2.2 Task 2: Improve the Representation of Boundary Layer Processes

Emissions of NO_x, VOC, and SO_2 from point and other (ships, helicopters) sources released over the outer continental shelf regions can be transported by land and sea breezes, leading to increased pollutant concentrations in coastal and inland regions surrounding the Gulf of Mexico. Because marine boundary layer processes are controlled mostly by weak forcing mainly due to shear production and in part by weak buoyancy production of turbulence, it is critical to study the benefits of using a turbulent kinetic energy-based scheme (TKE scheme) in the MM5 compared to a traditional eddy diffusivity-based first-order atmospheric boundary layer (ABL) scheme. We will perform MM5 simulations using a TKE-based scheme and an eddy diffusivity-based scheme and evaluated them rigorously in their ability to realistically simulate marine and coastal circulations**.**

1.2.3 Task 3: Assimilation of Surface Observations to Improve MM5 Simulations

At least, two types of surface observations are available for use in the MM5 simulations: traditionally available measurements from routine land-based measurements (at 2 m and 10 m AGL), and remotely sensed satellite-based observations. To a larger extent, both of these observations are mainly used for model evaluation rather than for improving model simulations.

1.2.3.1 Land-Based Observations

Since uncertainty in the specification of vegetation and soil parameters and other modeling assumptions and descritizations leads to modeling errors, particularly near the surface, we will use the Flux-Adjusting Surface Data Assimilation System (FASDAS) developed and tested by Alapaty et al. (2001a,b,c) to reduce these errors. In this continuous surface data assimilation technique, abundant land-based surface measurements of temperature and relative humidity (dew-point temperature) are used to nudge a 1-D model's lowest-layer air temperature and moisture along with the ground/skin temperature. To do this, surface-layer temperature and water vapor mixing ratio are directly assimilated by using the analyzed surface data, while ground/skin temperature and soil moisture are indirectly assimilated, thereby maintaining greater consistency between the soil temperature and moisture fields and the surface-layer mass-field variables. The FASDAS then uses the differences between the observations and model predictions to estimate adjustments to the surface fluxes of sensible and latent heat. These adjustment fluxes are then applied in calculating a new estimate of the soil/ground temperature and soil moisture for each soil layer using a land surface model (Chen and Dudhia, 2001), thereby affecting the predicted surface fluxes in the subsequent time step. This indirect data assimilation is applied simultaneously with the direct assimilation of surface data in the model's lowest layer, thereby maintaining greater consistency between the ground temperature and the surface layer mass-field variables. Usage of this technique is critical for minimizing errors in the ground temperature and

temperature gradients across coastal regions for realistic simulation of land-sea breeze circulations.

1.2.3.2 Satellite-Based Observations

To successfully simulate land-sea breeze circulations, improved predictions of the ground/soil temperature alone are not sufficient. One also needs to improve the representation of temperature gradients across the water-land continuum, resulting in more accurate representation of sea surface temperatures (SSTs). For this purpose, we have acquired satellite measurements from NOAA at very high spatial (1-km) and temporal (1-h) resolutions (http://www.mslabs.noaa.gov/cwatch/) over the Gulf of Mexico region. These satellite observations are ingested into the MM5 inputs in place of analyzed SSTs obtained at 40-km resolution. Preliminary results obtained from the MM5 simulations using the 40-km resolution analyzed SSTs and the satellite-based SSTs are presented in the Section 2.

1.2.4 Task 4: Simulate Mesoscale Circulations Using the MM5

We will perform and analyze MM5 simulations at various grid resolutions (i.e., 36, 12, and 4 km) under Tasks 2 and 3. We will then perform rigorous evaluations of the MM5 simulations. Finally, we will reconfigure the MM5 using the combination of schemes/methods that produces the best representation of atmospheric circulations in various domains. At that point, we will be ready to perform the final MM5 simulations using grid resolutions of 36, 12, and 4 km, which will be used to drive the MAQSIP-VGR for the time periods selected in Task 1. Results obtained from this comprehensive evaluation of MM5 simulations will be documented in our first annual report.

1.2.5 Task 5: Develop Emission Estimates

A variety of recent emission inventories and activity data will be used to prepare updated emissions inputs that are compatible with the MAQSIP-VGR. Existing emissions estimates from offshore area sources, consisting of commercial marine vessels and helicopter flights throughout the Gulf of Mexico, will be included in runs performed with our emissions modeling system, the Sparse Matrix Operator Kernel Emssions (SMOKE) system. We will also include the newest yearly emissions inventory being prepared by the Minerals Management Service (MMS), data from the Gulf wide Offshore Activities Data System (GOADS), and data that were collected in the Breton Offshore Activities Data System (BOADS). Processed emissions will be quality assured for correctness and accuracy, using various tools we have developed for this process; for example, we will compare “before” and “after” emissions totals against inventory data, and will examine temporal profiles to check their correctness. In addition, we will adapt SMOKE to accommodate the varying horizontal resolution of the MAQSIP-VGR grids.

1.2.6 Task 6: Enhance Representation of Cloud Processes in the MAQSIP-VGR

There are four primary processes by which clouds modify atmospheric chemical composition and distribution: (1) subgrid-scale vertical turbulent redistribution of mass; (2) aqueous chemical effects, including dissolution, dissociation, and kinetic reactions; (3) rainout and wet removal due to precipitation; and (4) modification of solar actinic flux and hence the rate of photolytic

reactions. The current representation of cloud effects in the MAQSIP-VGR accounts only for attenuation of photolysis rates due to the presence of clouds and is based on the cloud fields specified by the driving meteorological fields. In Task 6 we will extend the model representation of cloud processes to include the other affects discussed above by adapting the mesoscale and urban-scale cloud modules available in the regular grid version of the MAQSIP model. This includes representation of shallow convection, deep convection, resolved-scale clouds, and subgrid-scale layer clouds (McHenry and Binkowski, 1996; McHenry et al., 1996).

1.2.7 Task 7: Perform Simulations and Evaluation of the MAQSIP-VGR over the Houston-Galveston Domain

During the project year 2, we will use the MAQSIP-VGR to simulate the two 5-day periods chosen in Task 1 (during August-September 2000) over the Houston-Galveston domain. The availability of specialized measurements from the Texas 2000 air quality study provides a unique opportunity not only to conduct a detailed evaluation of the model but also to use both the model and the measurements in a complementary manner to improve our understanding of the complex coupling between dynamical and chemical processes that lead to rapid O_3 formation in the region. In the upcoming months we will also study how land-sea breeze circulations shape the distributions of primary and secondary species. Model simulations will focus on assessing the impact of onshore emissions from petrochemical industries on air quality in the region. Of particular interest is investigating the suitability of current emission inventories for representing emissions variability from these onshore facilities and consequently their potential impact on O_3 distributions.

1.2.8 Task 8: Perform Simulations and Evaluation of the MAQSIP-VGR over the Northeast Gulf Domain

During the second year of the project, we will perform MAQSIP-VGR simulations for selected periods during 1998 and/or 2000 over the northeast Gulf domain (the D04 southern Louisiana region in Figure 1). Model simulations will focus on assessing the impact of offshore emissions from oil and gas E&P facilities on local and regional air quality in the southern states. Model simulations of ozone will be compared to available measurements from the Aerometric Information Retrieval System (AIRS) (US EPA;http://www.epa.gov/air/data/index.html) database.

Section 2: Results and Discussion

We have completed various portions of the research outlined in Section 1. Some of the preliminary results obtained are presented below.

2.1 Develop Modeling Domains and Case Studies (Task 1)

Part of this task was completed during the first half of the project's first year as we have finalized the domains of numerical simulations. Our research is focusing on two domains: one over the

Houston-Galveston region and the other over southern Louisiana. For our numerical simulation case study over the Houston-Galveston region, we selected an initial time period of 23 August to 2 September 2000. These dates were chosen because a severe air pollution episode occurred over the region at that time. MAQSIP-VGR simulations will be performed to study the effects of various onshore and offshore emissions on the air quality of the coastal environments (Task 7). During the project's second year, we will perform final simulations of the MM5 for the entire period of 11 days after choosing the best modeling configuration, based on results obtained from several MM5 simulations. For the southern Louisiana region, we will select a time period pertinent for simulating ozone and aerosol concentrations during the second year of the project, also using the best configuration.

2.2 Improve the Representation of Boundary Layer Processes (Task 2)

In our previous report, we presented some results obtained by using the two different atmospheric boundary layer (ABL) schemes (i.e., the "Mrf" and "Eta" schemes) in order to study their ability to simulate regional circulations, precipitation, and other relevant parameters that control air pollution processes. We used the 36-km grid resolution in these simulations. Preliminary results reported in the previous report, briefly, were as follows: (1) Analysis of several soundings at various observational times revealed that at 0000 UTC the "Eta" temperature simulations were about 0.5 K closer to observations than that in the "Mrf", while at 1200 UTC the "Mrf" and "Eta" temperature simulations were similar to each other**,** (2) For water vapor mixing ratio, simulations by "Eta" seemed to be slightly higher than the measurements (~1 g/kg), while "Mrf" simulations showed slightly lower values (~-0.5 g/kg) than the observations. (3) Wind profiles showed some large errors in the directional component for the coastal regions in both the "Mrf" and "Eta" simulations, particularly in the ABL, while aloft wind speed and direction were very close to the observations for both "Mrf" and "Eta".

For the 36-km grid resolution simulations during the second half of the first project year (this reporting period), we developed precipitation analysis diagrams for comparison with those developed by the Climate Prediction Center (referred to as CPC) (see http://www.cpc.ncep.noaa.gov). The CPC dataset is derived from three sources: daily co-op stations from the National Climatic Data Center, the CPC dataset including data from the River Forecast Centers, and daily accumulations from an hourly precipitation dataset. There are about 13,000 station reports each day. The data were quality controlled to eliminate duplicates and overlapping stations, and standard deviation and buddy checks were applied. Then they were gridded into 0.25^{o}x 0.25^{o} using a Cressman Scheme. Note that precipitation amounts and distributions over oceanic regions may not be reliable due to a lack of data and interpolation artifacts.

Further, we completed 12- and 4-km grid resolution simulations for the "Mrf" and "Eta" cases, and developed statistics for evaluating results obtained from these two cases. We also obtained GOES-based remotely sensed data, and during the project's second year these data will be used to evaluate cloud fractions and insolation simulated by the MM5 using the best modeling configuration. In all figures below showing time series, the observations are referred to as "Obs"

and the model results obtained using the two ABL schemes are referred to as "MRF" and "ETA". In the quantity "(M–O)", which is used in preparing many statistics such as bias, "M" represents the modeled value and "O" represents the observed/measured value of a variable. Thus, if (M–O) is positive, the model is overpredicting that variable, and if (M–O) is negative the model is underpredicting.

Figures 2a, 2b, and 2c show accumulated precipitation data analyzed by the CPC and values obtained from "Mrf", and "Eta", respectively, for a period of 24 h ending 1200 UTC 24 August 2000. In general, simulated precipitation is qualitatively very similar in "Mrf" and "Eta". Over the region of specific interest to this project, i.e., eastern Texas, "Eta" has led to more precipitation than in "Obs" (i.e., CPC) and "Mrf". The overall precipitation patterns in "Mrf" are marginally better than those in "Eta". Figures 3a, 3b, and 3c are analogous figures for a period of 24 h ending 1200 UTC 28 August 2000. Again, over the eastern Texas region, the "Eta" case overpredicted the precipitation when compared to "Obs" and "Mrf", even though the spatial distribution and rate are very similar.

Since 12-km grid resolution simulations are primarily used to provide lateral boundary conditions to 4-km grid resolution domains, and our focus is on model simulations using the high-resolution grids, we present evaluation results for the 4-km grids for "Mrf" and "Eta". Figure 4a shows the temporal variation of near-surface temperature (K) for "Obs", "Mrf", and "Eta". During this five-day period, observations indicated a warming-up trend. In general, both "Mrf" and "Eta" simulated this trend well, with the exception of the last day of simulation. "Mrf" and "Eta" both have a maximum cooler bias during the daytime maximum and nighttime minimum temperature occurrence period. Figure 4b shows the temporal variation of bias in near-surface temperature for "Mrf" and "Eta". In a general sense, "Mrf" has a lesser temperature bias (by about 1-2 K) compared to "Eta". The large positive bias present at about 36 h of simulation in both the cases is due to model's inability to simulate a thunderstorm that was observed during that time. This has led to an unrealistic heating due to the absence of modeled clouds at that time. Barring this incident, "Mrf" seems to be a better choice at least for temperature simulations. Figure 5a shows the temporal variation of bias for the near-surface water vapor mixing ratio (g/kg). For "Mrf", there exists a significant dry bias, particularly during the second and fourth days of simulation, as compared to "Eta", which has a moist bias during that time.

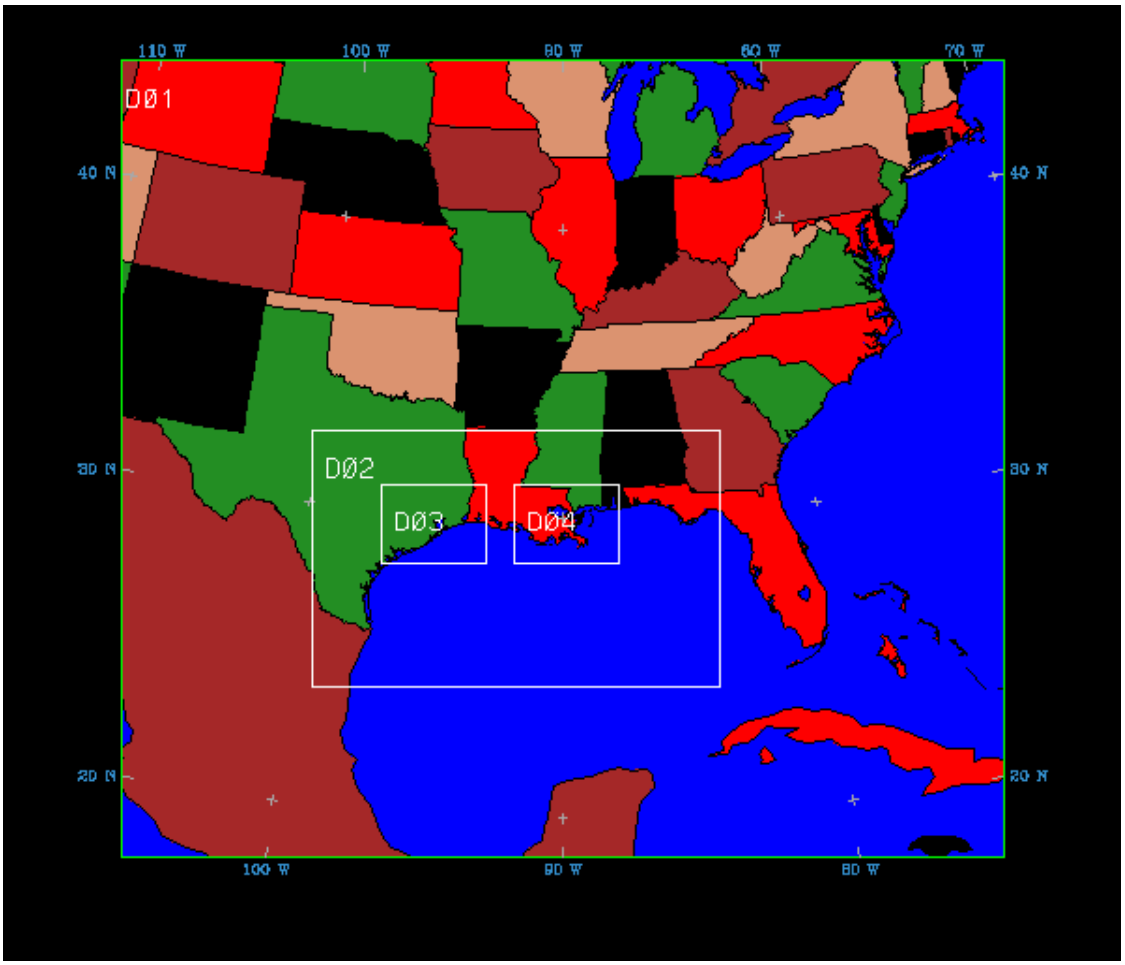


Figure 1. Simulation domains for the MM5 simulations. Domains D01 and D02 use 36- and 12-km grids, respectively, while domains D03 and D04 use 4-km grids located over the Houston-Galveston region and southern Louisiana.

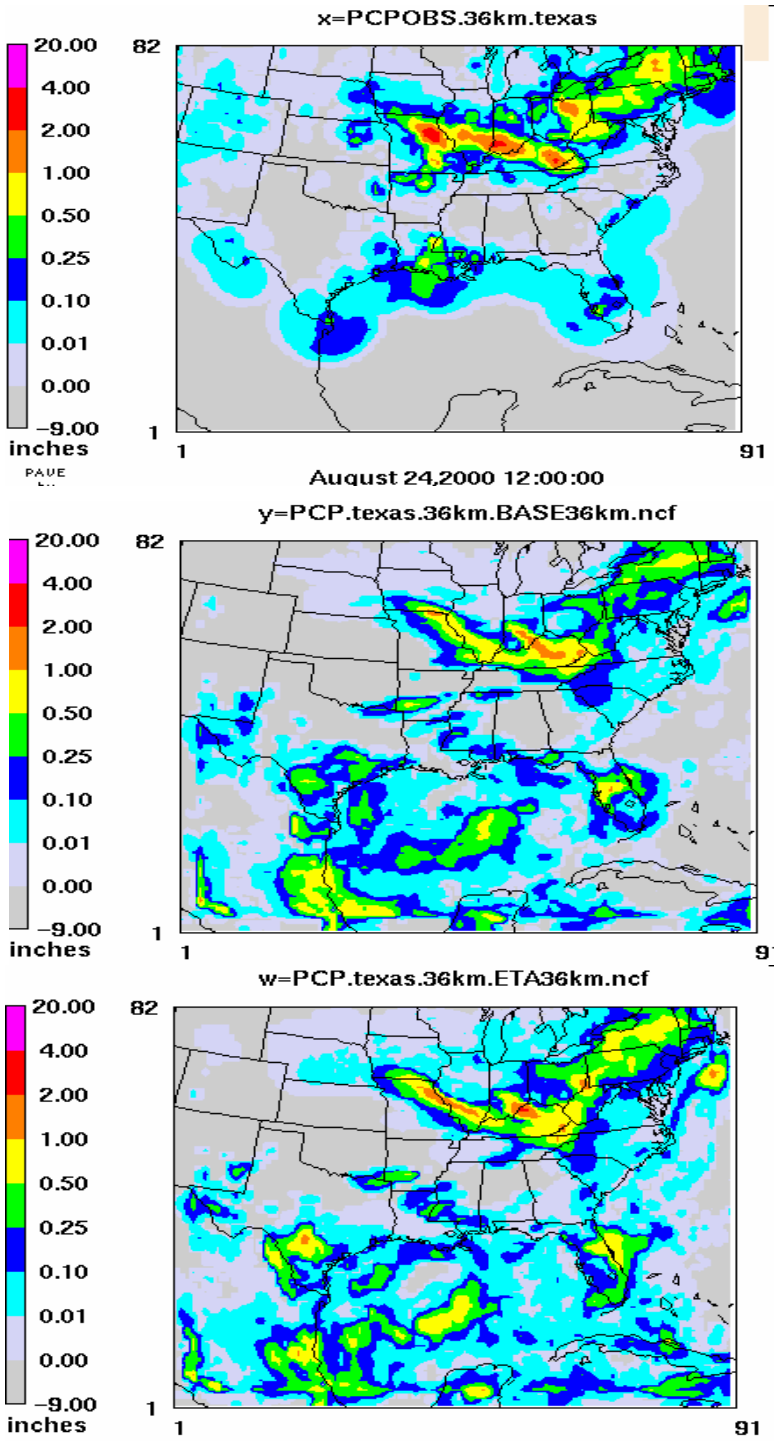


Figure 2. Accumulated precipitation (inches) for a period of 24 h ending at 1200 UTC 24 August 2000 from the (a) CPC anlaysis, (b) "Mrf", and (c) "Eta" cases.

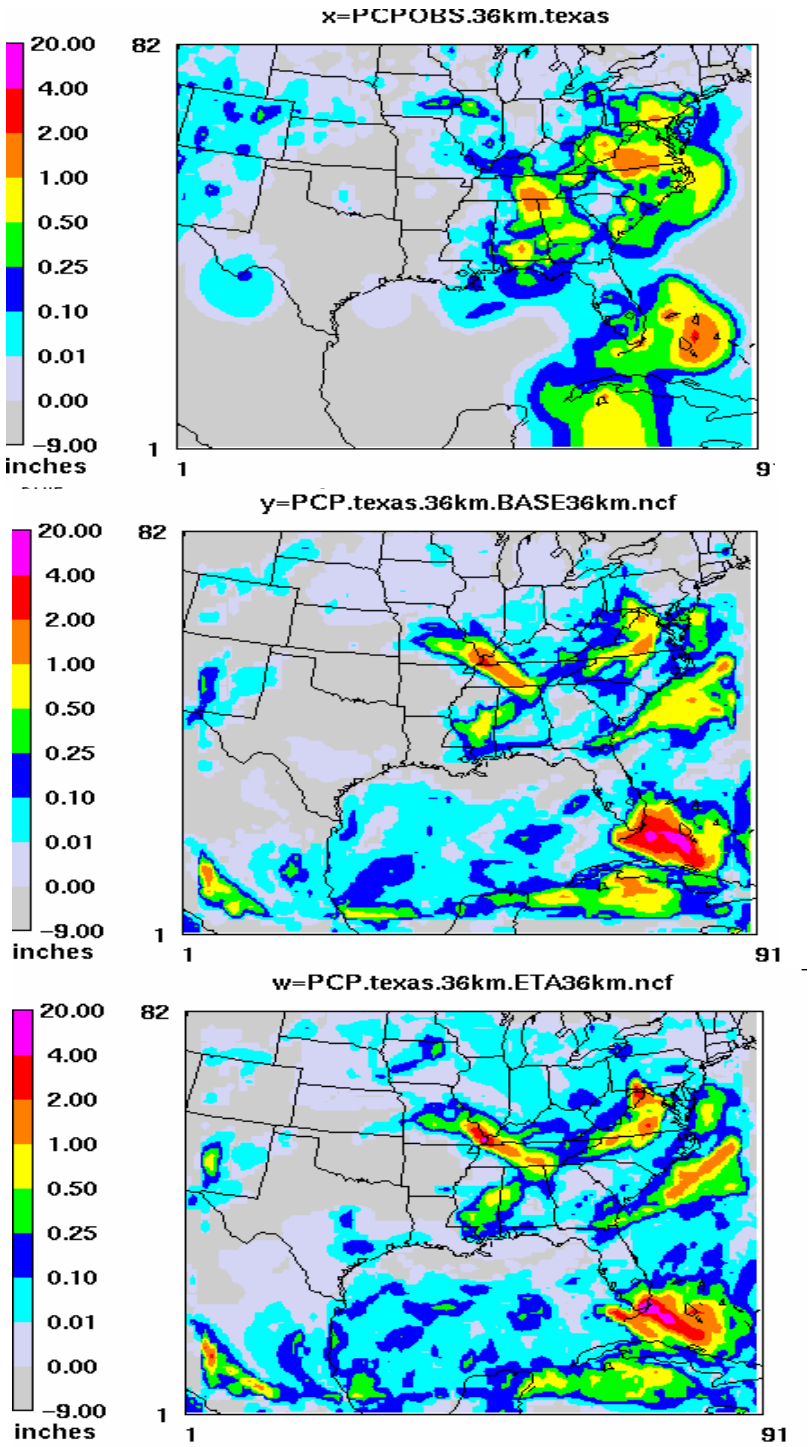


Figure 3. Accumulated precipitation (inches) for a period of 24 h ending at 1200 UTC 28 August 2000 from the (a) CPC anlaysis, (b) "Mrf", and (c) "Eta" cases.

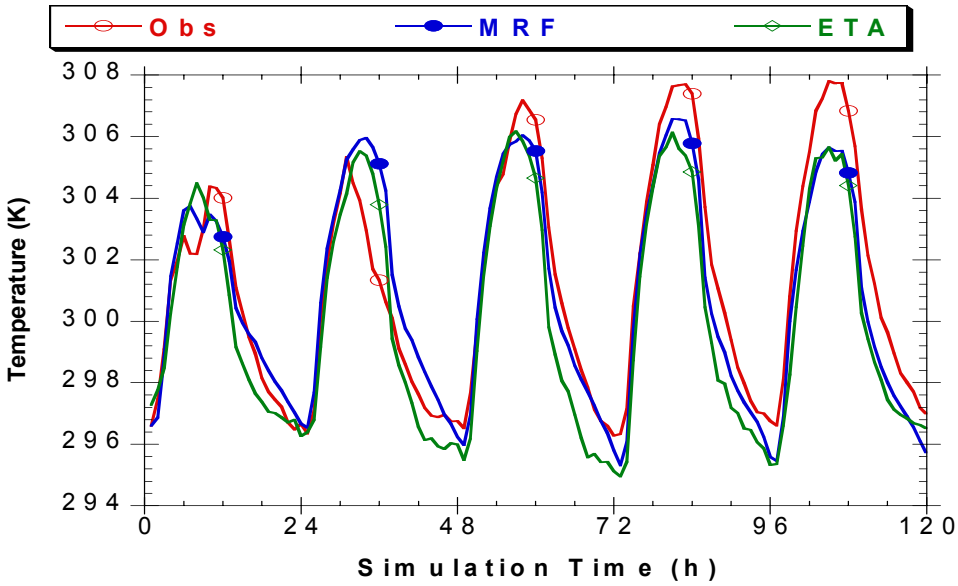


Figure 4a. Temporal variation of near-surface air temperature averaged over all of the measurements and corresponding modeled values, starting at 1200 UTC 23 August 2000 for the "Mrf" and "Eta" cases for 4-km grids.

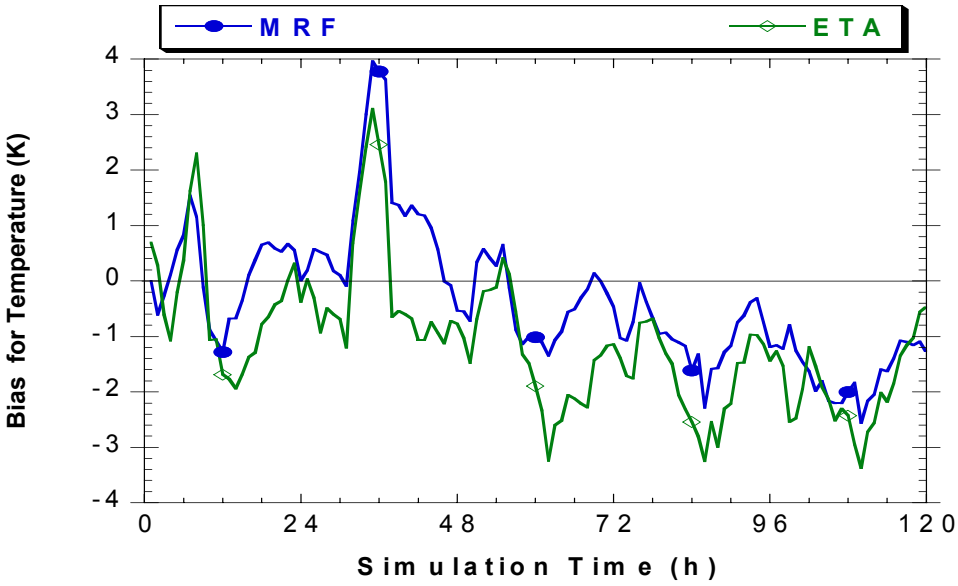


Figure 4b. Temporal variation of bias in the averaged near-surface air temperature for the "Mrf" and "Eta" cases, starting at 1200 UTC 23 August 2000.

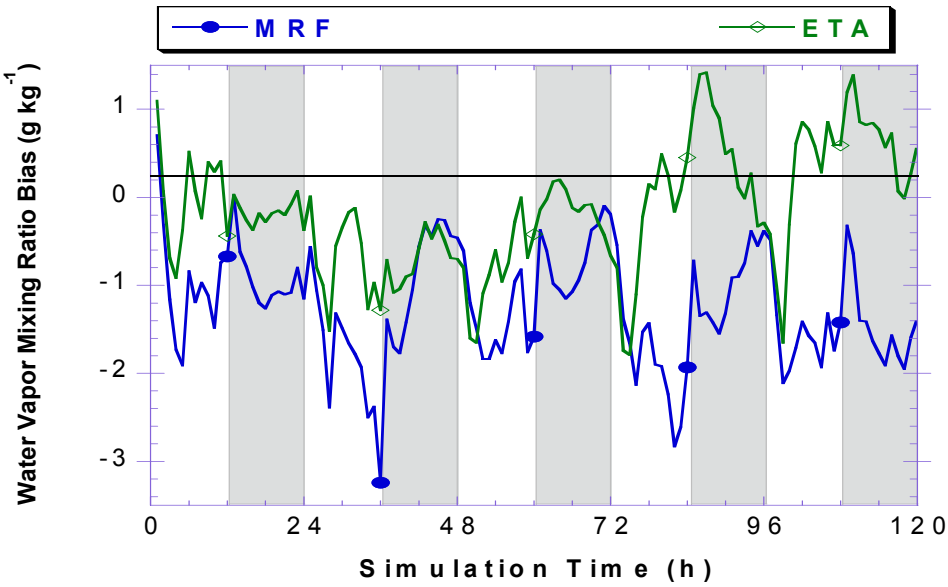


Figure 5a. Temporal variation of bias in the averaged near-surface air water vapor mixing ratio for the "Mrf" and "Eta" cases, starting at 1200 UTC 23 August 2000.

Similar results are found in the root mean square errors (RMSEs) shown in Figure 5b. To find out the main reasons for the presence of large RMSEs in "Mrf", we intercompare the modeled simulated precipitation amounts and spatial distribution with those from the the CPC precipitation analysis shown in later figures. Figures 6a and 6b indicate the temporal variation of RMSE for near-surface wind speed and its direction. In the "Eta" case, the RMSEs are smaller compared to those in the "Mrf" case. However, errors in the wind direction are smaller in "Mrf" compared to those in "Eta". Figure 7a shows the accumulated total precipitation from CPC for a period of 24 h ending 1200 UTC 24 August 2000. Figures 7b and 7c show modeled accumulated total precipitation for the same period as in the CPC analysis for the "Mrf" and "Eta" cases, respectively. It can be seen that "Eta" leads to overprediction of precipitation as compared to "Obs" (i.e., CPC) and "Mrf". This leads to spurious cloud cover affecting the photolysis rates, which play an important role in the ozone formation during the daytime. A similar result was also found for the precipitation during the rest of the simulation days; as an additional analysis, we present the accumulated precipitation ending at 1200 UTC 28 August 2000 in Figures 8a, 8b, and 8c for the 4-km grids. Again, there is a strong indication of spurious precipitation in "Eta" while "Obs" and "Mrf" indicate near-clear sky conditions.

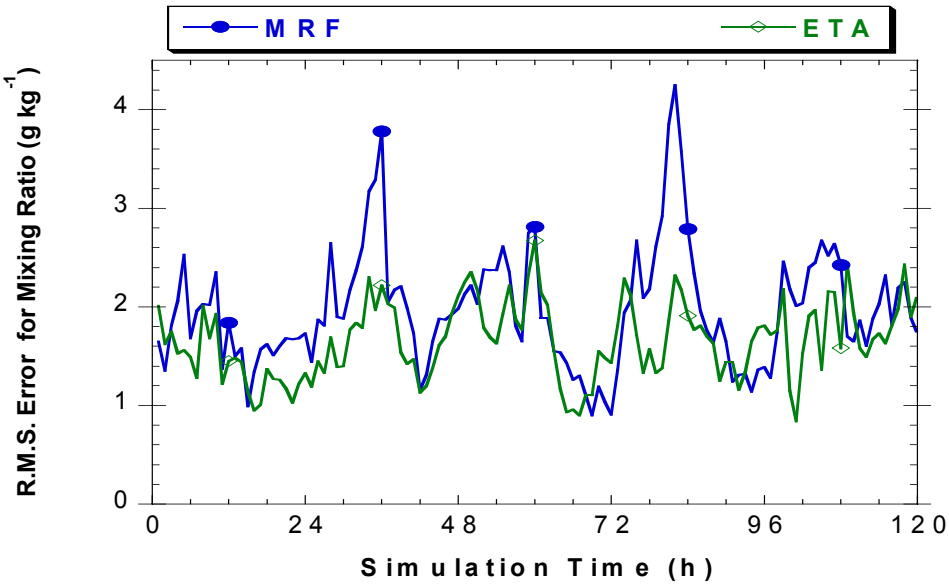


Figure 5b. Temporal variation of root mean square errors in the averaged near-surface air water vapor mixing ratio for the "Mrf" and "Eta" cases, starting at 1200 UTC 23 August 2000.

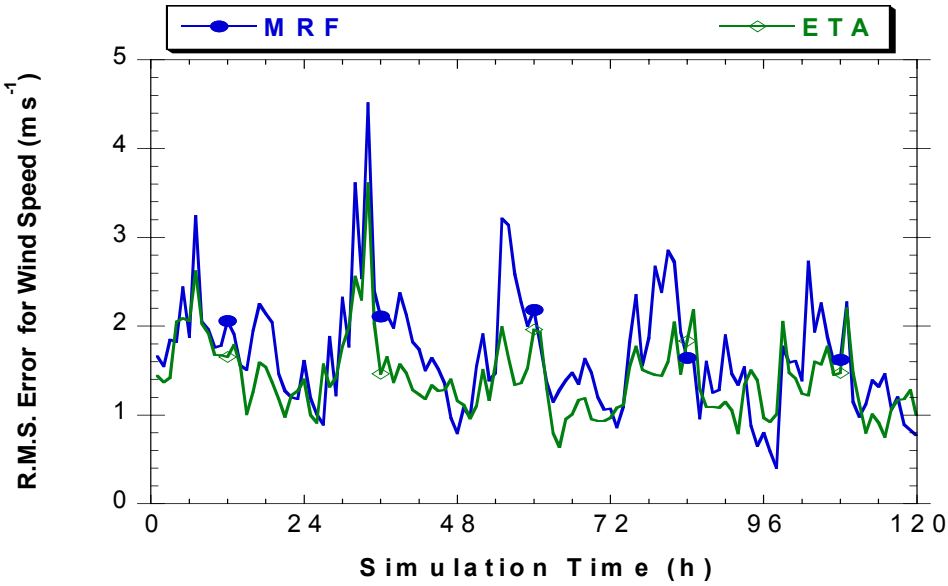


Figure 6a. Temporal variation of root mean square errors in the averaged near-surface horizontal wind speed for the "Mrf" and "Eta" cases, starting at 1200 UTC 23 August 2000.

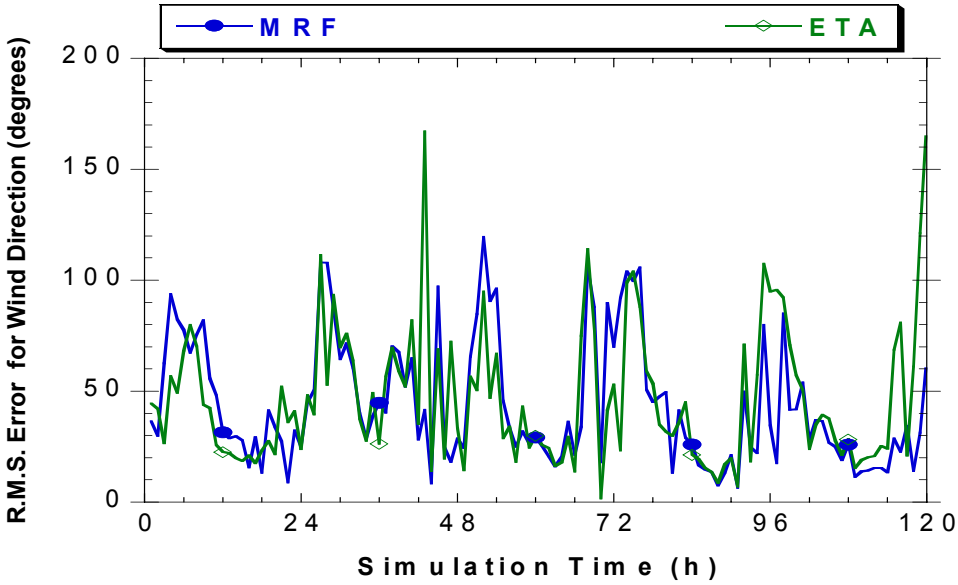


Figure 6b. Temporal variation of root mean square errors in the averaged near-surface horizontal wind direction for the "Mrf" and "Eta" cases, starting at 1200 UTC 23 August 2000.

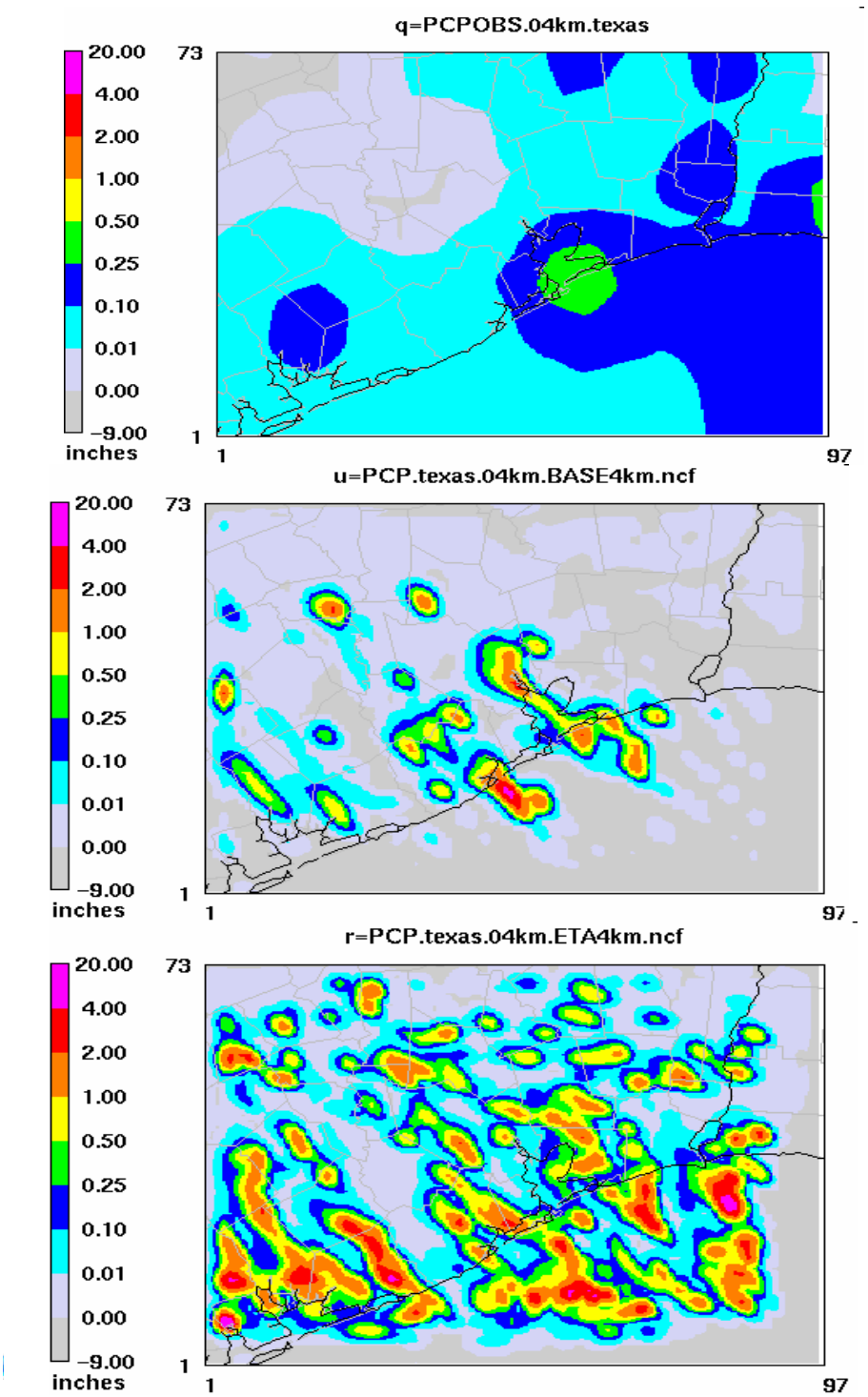


Figure 7. Accumulated precipitation for the (a) "Obs", (b) "Mrf" and (c) "Eta" cases, ending at 1200 UTC 24 August 2000.

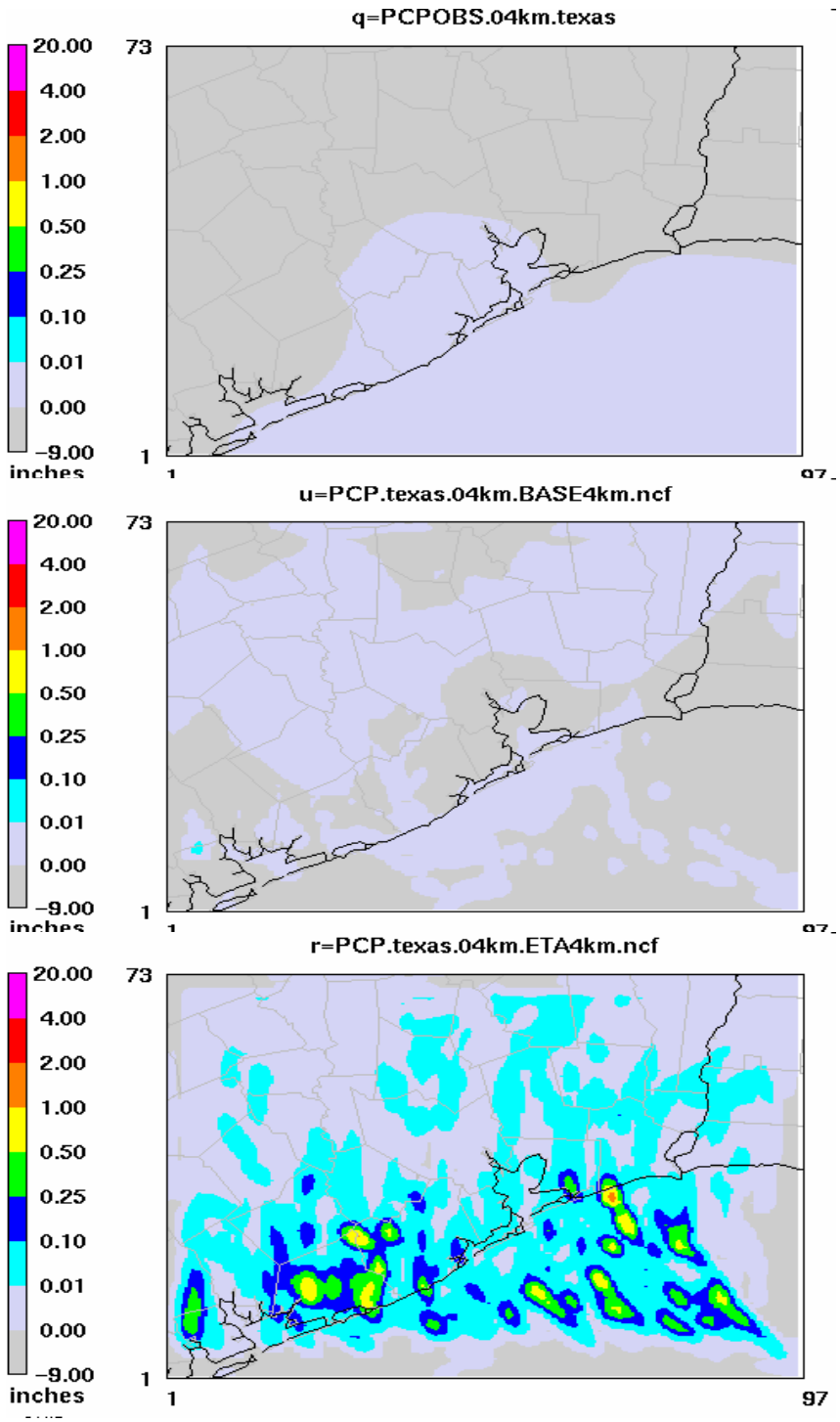


Figure 8. Accumulated precipitation for the "Obs", "Mrf" and "Eta" cases, ending at 1200 UTC 28 August 2000.

In general, the temperature and wind speed simulations in "Eta" compare well with observations, while the mixing ratio and wind directions simulated by "Mrf" compare well with observations. However, precipitation is overestimated in "Eta" while slightly underestimated in "Mrf". For these reasons, we strongly believe that the "Mrf" simulations, in general, are usable to drive the air quality model. We will therefore utilize the "Mrf" simulations as meteorological inputs to drive the MAQSIP-VGR.

2.3 Assimilation of Surface Observations to Improve MM5 Simulations (Task 3)

2.3.1 Assimilation of Land-based Surface Observations using the FASDAS

Modeling errors in simulated ABL parameters can significantly affect the outcome of an air quality simulation. To alleviate such modeling errors, surface observations can be used to improve the accuracy of the simulated ABL in a meteorological model. We will do this using the Flux-Adjusting Surface Data Assimilation System (FASDAS) introduced in Section 1.2.3.1. The advantage of this technique over others is that the soil moisture assimilation is directly based on the size of the errors in the surface layer water vapor mixing ratio. We believe that our FASDAS method is the first of its kind in mesoscale modeling capable of using surface data for minimizing modeling errors.

During the first half of the project's first year**,** we implemented the FASDAS into the MM5 using a sophisticated land-surface model (Chen and Dudhia, 2001) and the MRF boundary layer scheme. After successful implementation, we performed a test simulation using the same 36-km grid employed in Section 2.2, using the FASDAS and compared with the "Base" simulations and these are described in our previous semiannual project report. One of the reasons for using the MRF scheme as a default ABL scheme in the MM5 simulations is the fact that it is the most widely used scheme. In our previous report, we provided some preliminary analysis and evaluation of the results obtained using the FASDAS technique in the MM5. The MM5 simulations using the MRF scheme discussed in Section 2.2 were referred to there as "Mrf". Here, for convenience, we refer to those same results obtained from the MRF as "Base", while the MM5 results obtained using the FASDAS will be referred to as "Fasdas".

We acquired the CPC analyses for precipitation and compared them with the model simulations for the 36-km grids. Figures 9a, 9b, and 9c show the accumulated precipitation ending at 1200 UTC 24 August 2000 for "Obs", "Base", and "Fasdas". The spatial distribution of precipitation in "Base" and "Fasdas" in general is very similar, with higher totals in "Fasdas". Over eastern Texas, both cases (i.e., "Base" and "Fasdas") overpredicted the precipitation estimates compared to observations. Analyzed and simulated precipitation totals for another 24 h, ending at 1200 UTC 28 August 2000, are shown in Figures 10a, 10b, and 10c. Observations indicated no traceable precipitation over southern and eastern Texas, while "Base" indicated trace amounts of precipitation covering southern Texas. In "Fasdas", while no precipitation was simulated in the region immediately surrounding the Houston-Galveston area, south and north of it there exists an accumulated precipitation of about 0.1" that is not supported by observations. Analysis of precipitation distribution and magnitudes for the other days of simulation indicated mixed

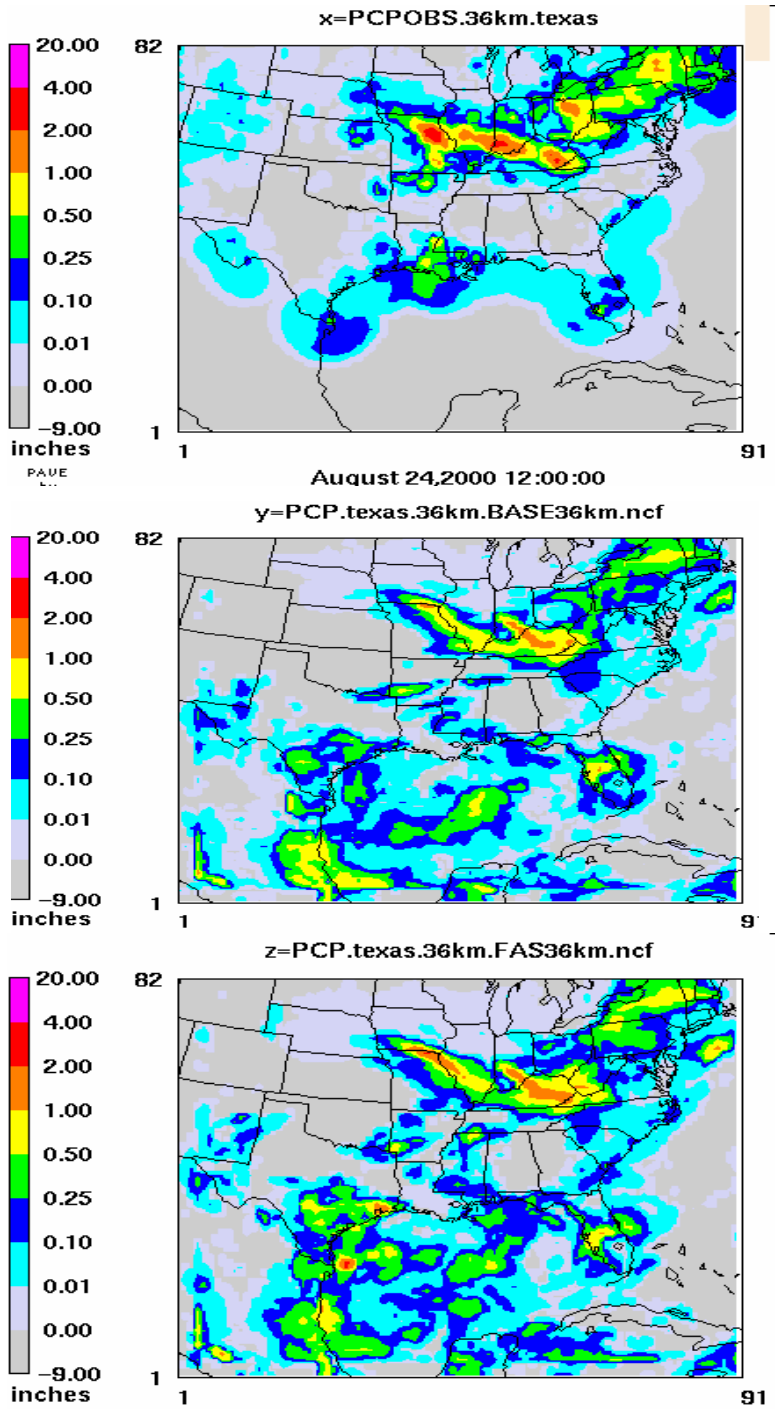


Figure 9. Accumulated precipitation (inches) for a period of 24 h ending at 1200 UTC 24 August 2000 from the (a) CPC anlaysis, (b) "Base", and (c) "Fasdas" cases.

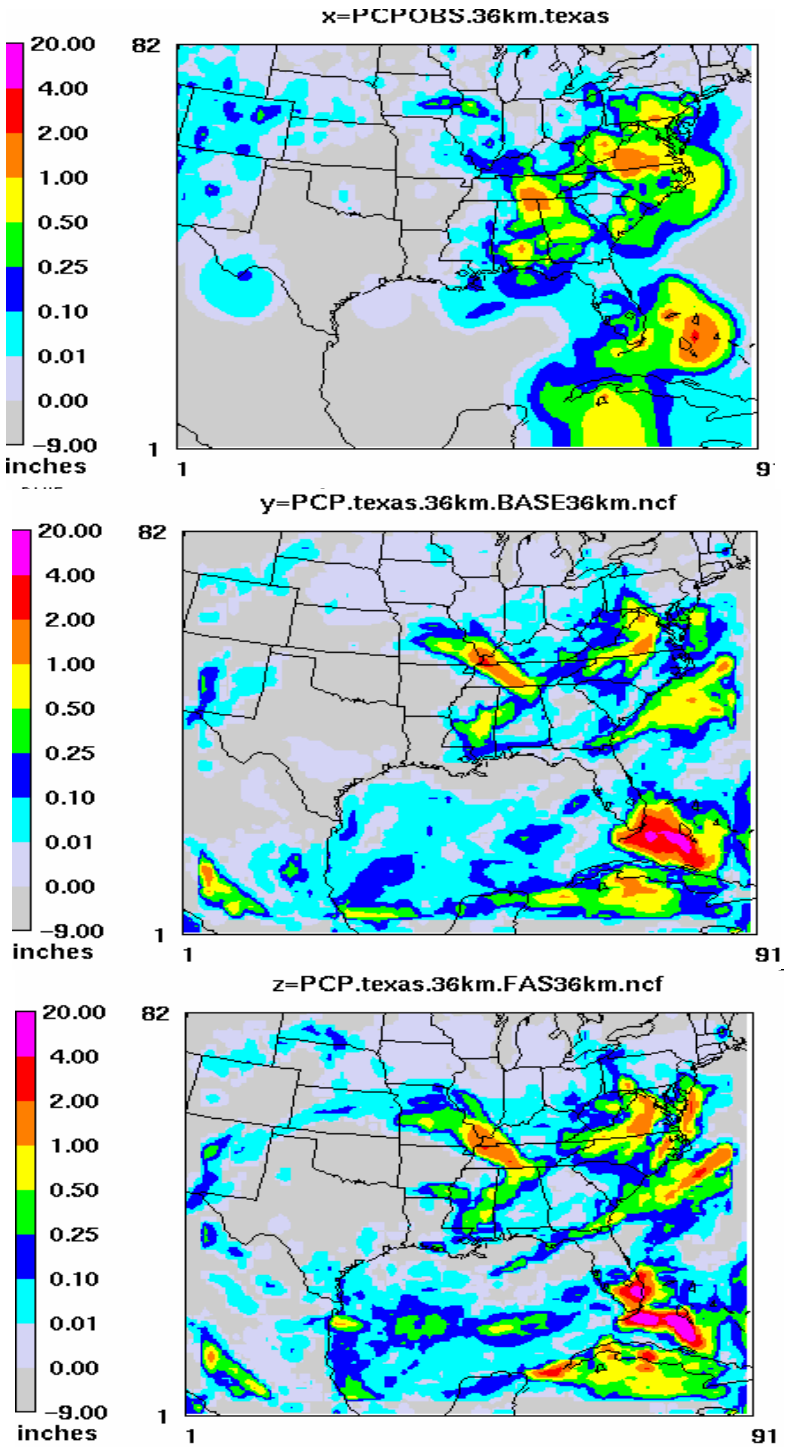


Figure 10. Accumulated precipitation (inches) for a period of 24 h ending at 1200 UTC 24 August 2000 from the (a) CPC anlaysis, (b) "Base", and (c) "Fasdas" cases.

results; "Base" and "Fasdas" showed marked similarities and differences when compared to observed precipitation over different regions. We now present a statistical evaluation of 4-km grid model simulations for "Base" and "Fasdas". There are about 15 surface measurements available in the 4-km domain, and one upper-air sounding. These measurements, along with the CPC precipitation analysis, are used to evaluate the "Base" and "Fasdas" cases.

Figure 11a shows the temporal variation in the ~2 m AGL air temperature from "Obs", "Base", and "Fasdas" for the 4-km grid simulations. Both "Base" and "Fasdas" indicate similar magnitudes and temporal variation, with a small improvement in "Fasdas".

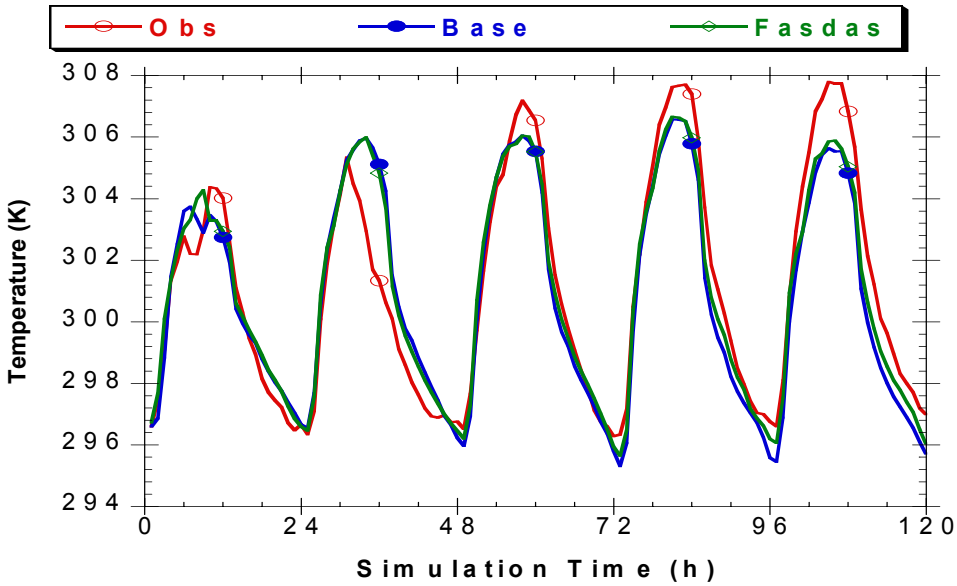


Figure 11a. Temporal variation of near-surface air temperature averaged over all of the measurements and corresponding modeled values, starting at 1200 UTC 23 August 2000 for the "Base" and "Fasdas" cases for 4-km grids.

Prediction of cooler temperatures by both of them is caused mainly by reduced insolation due to cloud cover (not shown). Similar results can be found in the RMSE distribution shown in Figure 11b, which indicates slightly improved performance by "Fasdas".

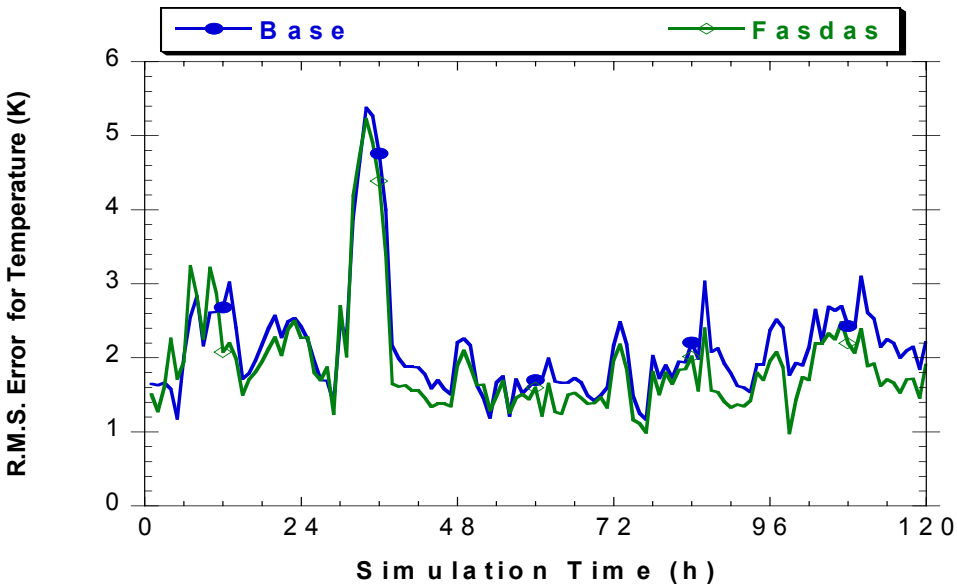


Figure 11b. Temporal variation of near-surface air temperature RMS errors for the "Base" and "Fasdas" cases using 4-km grids starting at 1200 UTC 23 August 2000 .

The temporal variation in the averaged near-surface water vapor mixing ratio for "Obs", "Base", and "Fasdas" is shown in Figure 12a and the RMSEs for these two cases are shown in Figure 12b. There is a marginal improvement in "Fasdas" compared to "Base". Figures 13a and 13b give the RMSEs in the simulated horizontal wind speed and its direction for the near-surface winds. There is a marginal improvement in "Base" compared to "Fasdas" for the wind speed, while there is not much difference in the wind direction simulations.

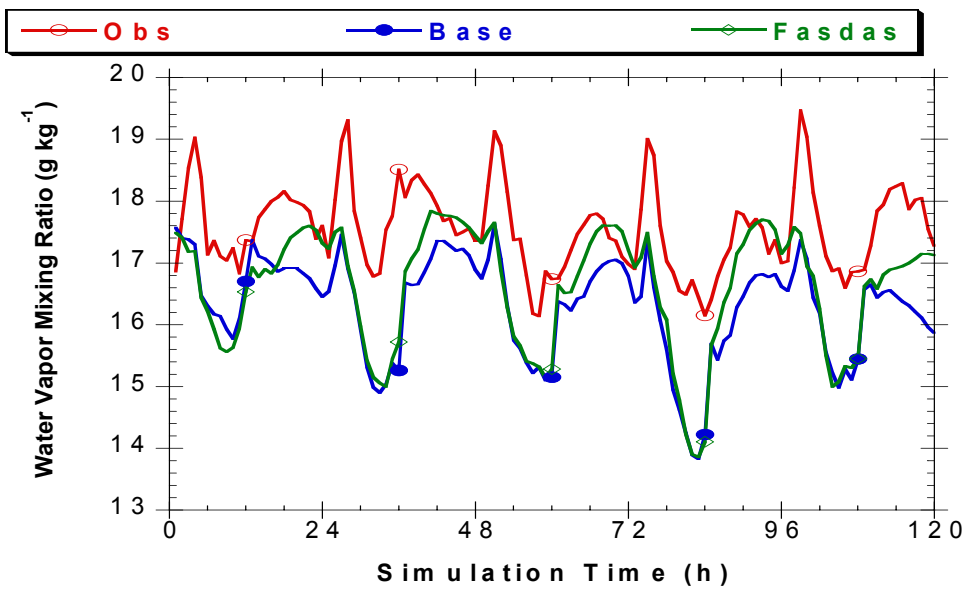


Figure 12a. Temporal variation of averaged near-surface air water vapor mixing ratio for the "Base" and "Fasdas" cases, starting at 1200 UTC 23 August 2000.

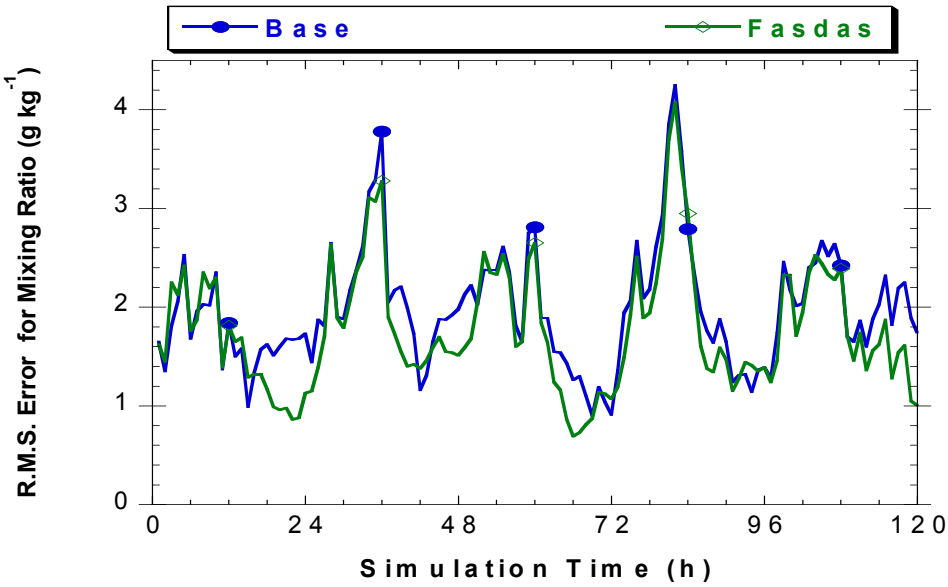


Figure 12b. Temporal variation of near-surface air mixing ratio RMS errors for the "Base" and "Fasdas" cases using 4-km grids starting at 1200 UTC 23 August 2000 .

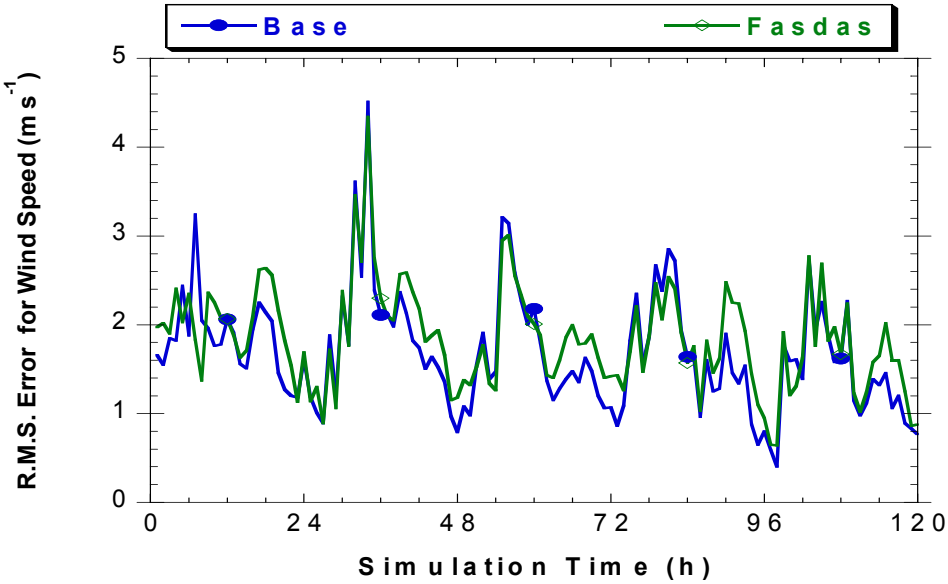


Figure 13a. Temporal variation of near-surface horizontal wind speed RMS errors for the "Base" and "Fasdas" cases using 4-km grids starting at 1200 UTC 23 August 2000 .

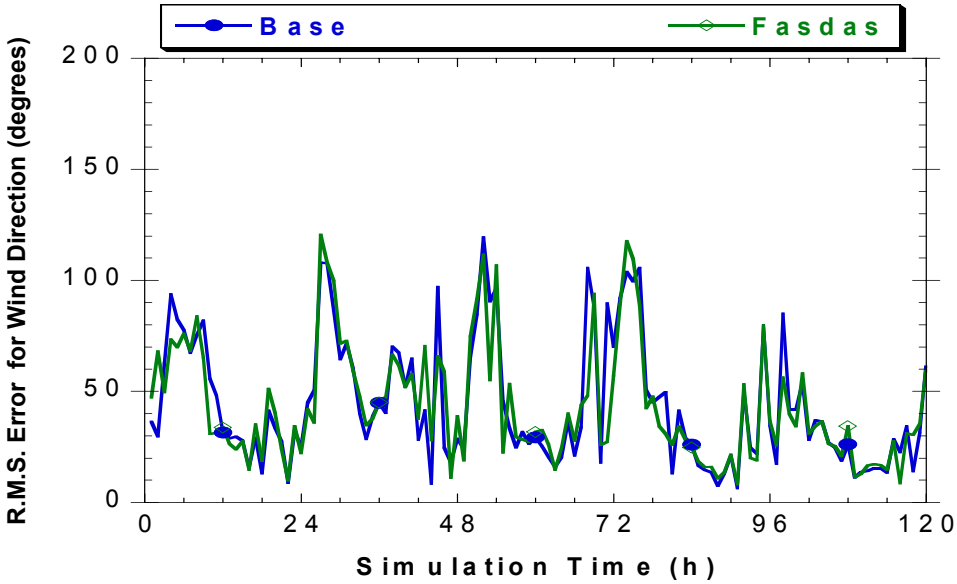


Figure 13b. Temporal variation of near-surface horizontal wind direction RMS errors for the "Base" and "Fasdas" cases using 4-km grids starting at 1200 UTC 23 August 2000 .

Figures 14a and 14b show the accumulated precipitation in "Obs", "Base", and "Fasdas" ending at 1200 UTC 24 August respectively. There are some minor differences between "Base" and "Fasdas" in the simulated precipitation, with higher magnitudes in "Fasdas". Precipitation simulations for the period ending 1200 UTC 28 August also indicate insignificant differences between "Base" and "Fasdas". In general, these simulations qualitatively compare well with the CPC analysis, i.e., "Obs".

We further examined the single sounding present in the simulation domain and compared with the measured soundings for several periods of model simulation. These analyses indicated that the "Base" and "Fasdas" soundings for temperature, moisture, and winds showed virtually no differences between them. The main reason for these results is that there are no surface measurements available in the neighborhood of the sounding measurements, hence no improvements were found over this region.

Note that only about 10 surface measurements are available for use by the FASDAS to correct the modeling errors out of about 7000 grid points. Thus, very minor improvements are expected in "Fasdas" for the 4-km grids, as opposed to the 36-km grids, where about 800 surface measurements are used in "Fasdas". In the future, we may include additional special observations that may be available from the Texas 2000 Air Quality Study to further improve "Fasdas" case simulations. In general, there are minor improvements in "Fasdas" compared to "Base" and hence we would like to utilize "Fasdas" in creating final meteorological fields in the final modeling configuration.

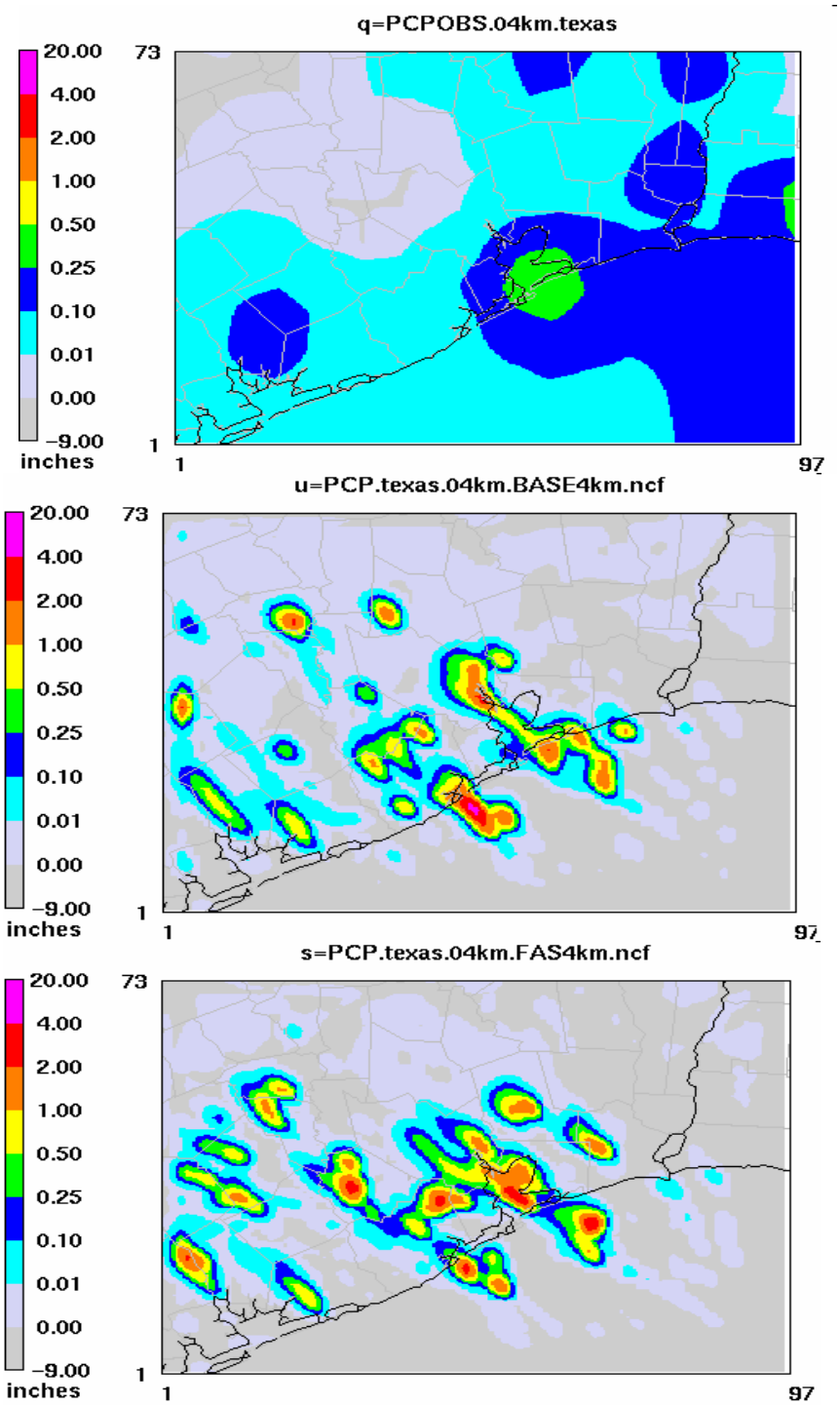


Figure 14a. Accumulated precipitation for the "Obs", "Base" and "Fasdas" cases, ending at 1200 UTC 24 August 2000 for the 4-km grids.

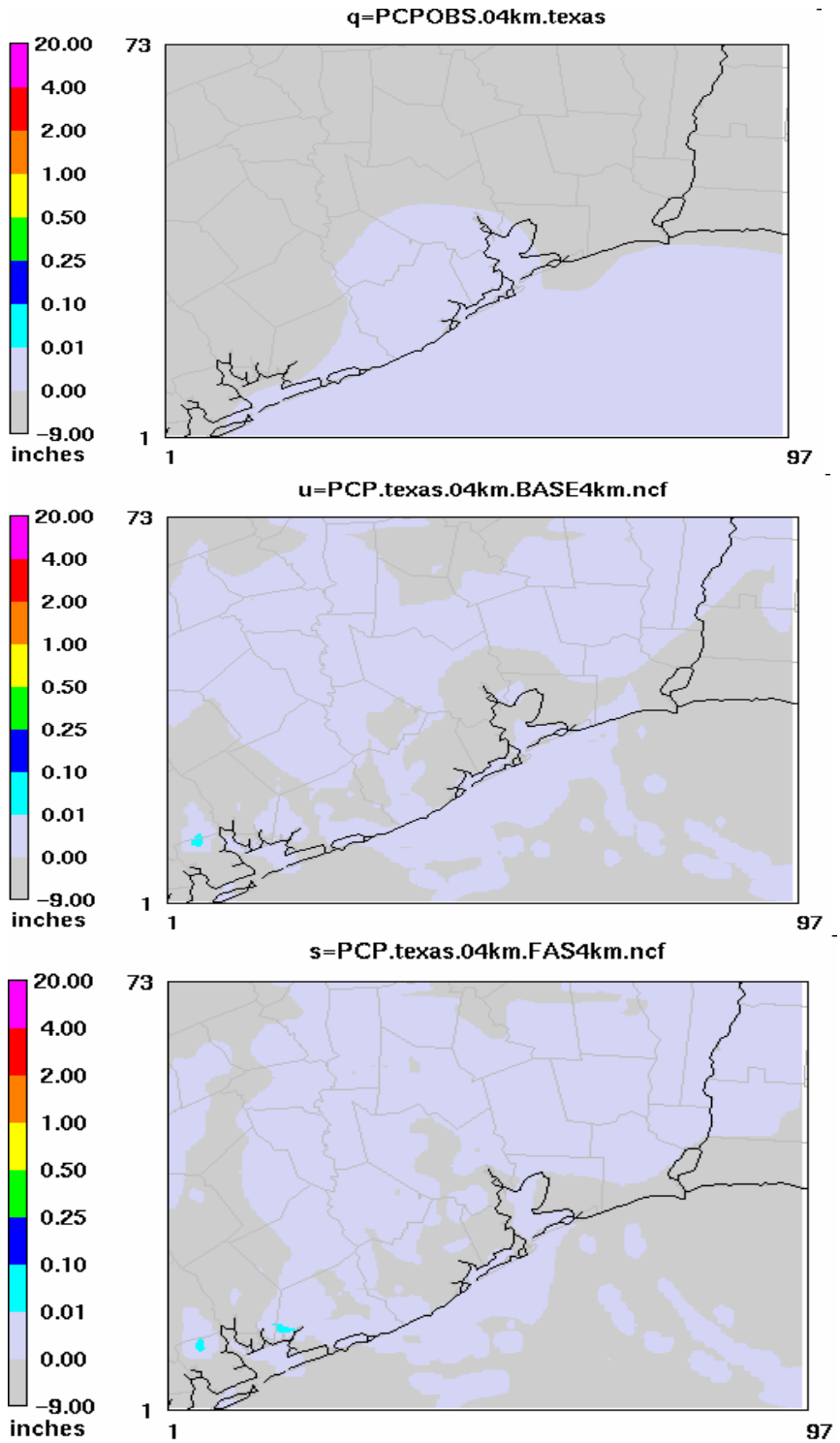


Figure 14b. Accumulated precipitation for the "Obs", "Base" and "Fasdas" cases, ending at 1200 UTC 28 August 2000 for the 4-km grids.

2.3.2 Ingestion of Satellite-Measured Sea Surface Temperatures into the MM5

Warm waters in the Gulf of Mexico are a major mesoscale feature influencing local weather, through land-sea breezes and precipitation events, particularly during warmer time periods. To realistically simulate meteorological and air quality features over the coastal environments, it is important to represent sea surface temperatures (SSTs) over the Gulf of Mexico. In the traditional approach for performing meteorological simulations, one normally uses the coarse-resolution SSTs available from the Eta Data Analysis System (EDAS) of the National Center for Environmental Prediction (NCEP) at 40-km resolution in prescribing sea surface temperatures over water-covered grid cells in a mesoscale model. However, this leads to a bulk representation of SSTs that could lead to some modeling errors, particularly over the coastal regions such as the Houston-Galveston region.

In the previous report, we described part of the research work completed under this task. During that period of research, we acquired remotely sensed SSTs at 4x4-km resolution archived by NOAA for a small region east of the Houston-Galveston area. We then performed some QA/QC procedures to weed out any missing or bad data (cloud pixels) and ingested the remotely-sensed SST data into the MM5 preprocesssing system for further processing and use in developing initial and lateral boundary meteorological fields for use by the MM5. Since we were able to acquire only partial data for the period of interest, the MM5 model simulations performed for the 36- and 12-km grids used only the traditional SST data (coarse NCEP data). For the 4-km grid we performed two MM5 simulations, one using the traditional SST data and the other using NOAA's satellite-derived SSTs. We believe that we may be the first researchers to ingest satellite-derived SSTs into the MM5 for use in an air quality modeling research effort. In the future, we will acquire remotely-sensed SSTs suitable for domains D01 (36-km grids) and D02 (12-km grids) and repeat these simulations for these two domains, then finally for the D03 and D04 domains (both 4-km grids).

Some preliminary analysis and diagnostic results were presented in the previous report. In this report, we present our evaluation results. Results obtained from using the analyzed SSTs and the satellite-derived SSTs are referred to in the text as "Base" and "Sat," respectively.

Figure 15a shows the temporal variation in the averaged 2-m AGL temperature from the measurements ("Obs") and from the "Base" and "Sat" cases. During the daytime, the maxima are well simulated in "Sat" compared to "Base", while during the nighttime a mixed results are seen for the minima when intercompared with "Obs". However, analysis of RMSEs (Figure 15b) indicates that daytime simulations with "Sat" are better (lower RMSEs), while during the nighttime the RMSEs in "Base" are relatively lower compared to "Sat". Analysis of temporal variation of near-surface water vapor mixing ratio and its RMSEs (Figures 16a and 16b) indicate again somewhat similar results, without any clear indication of which case is the better. Analyses of vertical soundings for temperature, dew point temperature, and horizontal wind vectors (Figures 17a and 17b) also indicate that both the "Base" and "Sat" cases do equally well when compared to observations. Finally, we consider the 24-h accumulated precipitation ending at 1200 UTC for 24 August and 28 August (Figures 18a and 18b, respectively). In the "Sat" case it appears that the accumulated precipitation is higher in magnitude and is in closer agreement with

"Obs", particularly over the Houston Bay area. With the exception of locally produced thunderstorms in "Base" and "Sat", these results are comparable to each other.

One of the main hindrances in analyzing 4-km grid simulations is the lack of statistically significant numbers of measurements that would allow a stronger conclusion on which case is performing better compared to the other. The diagnostic analysis presented in our previous report indicated the presence of larger differences between the "Base" and "Sat" cases. Considering all of these results, we believe that, in general, the "Sat" case seems to be performing better than the "Base" case, while noting the point that differences between both the simulations are very small for the parameters for which measurements are available.

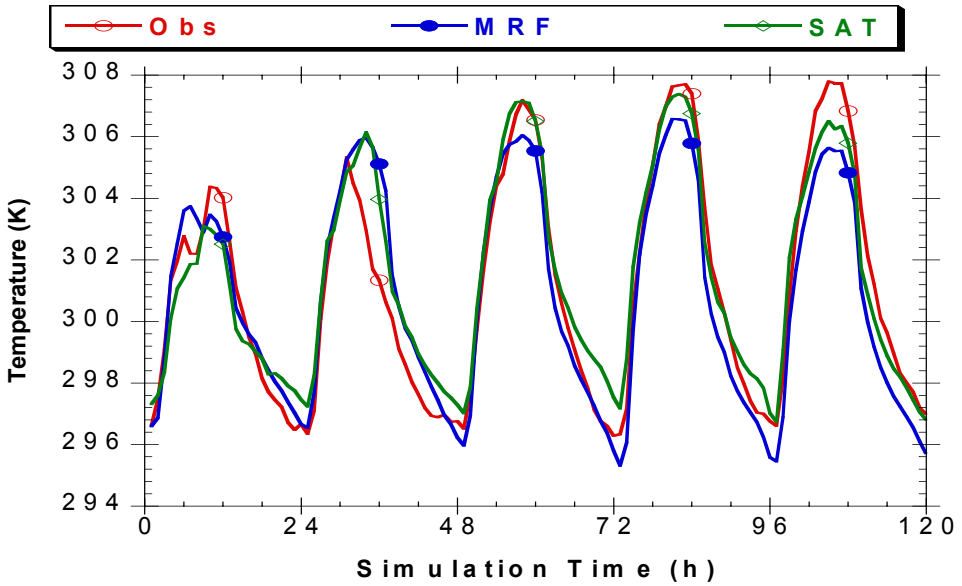


Figure 15a. Temporal variation of near-surface air temperature averaged over all of the measurements and corresponding modeled values, starting at 1200 UTC 23 August 2000 for the "Base" and "Sat" cases for 4-km grids.

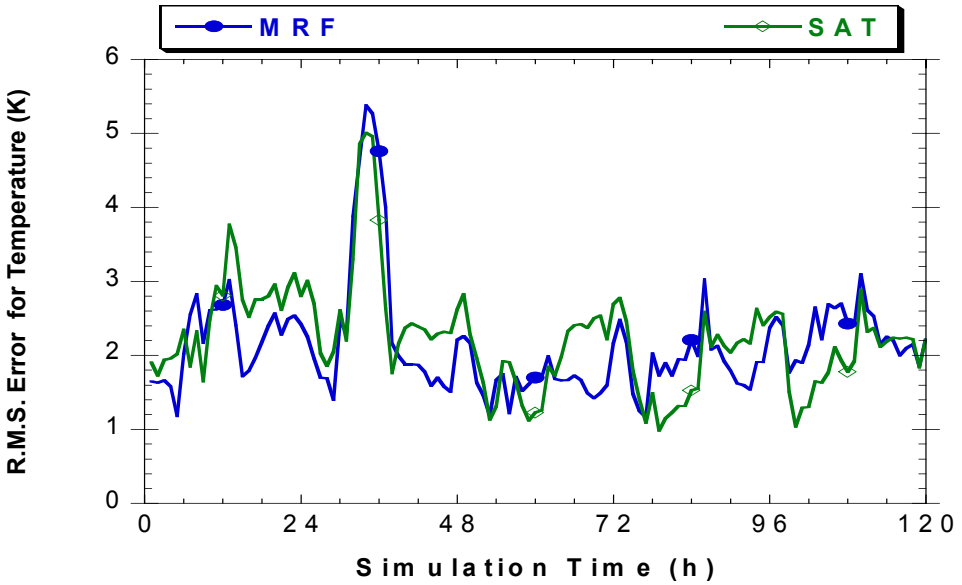


Figure 15b. Temporal variation of near-surface air temperature RMS errors for the "Base" and "Sat" cases using 4-km grids starting at 1200 UTC 23 August 2000 .

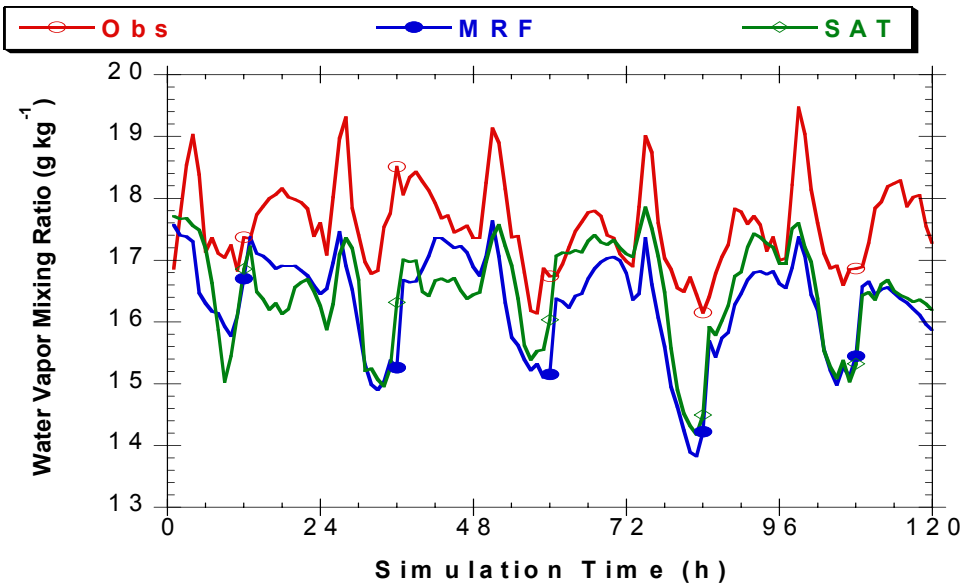


Figure 16a. Temporal variation of averaged near-surface air water vapor mixing ratio for the "Base" and "Base" cases, starting at 1200 UTC 23 August 2000.

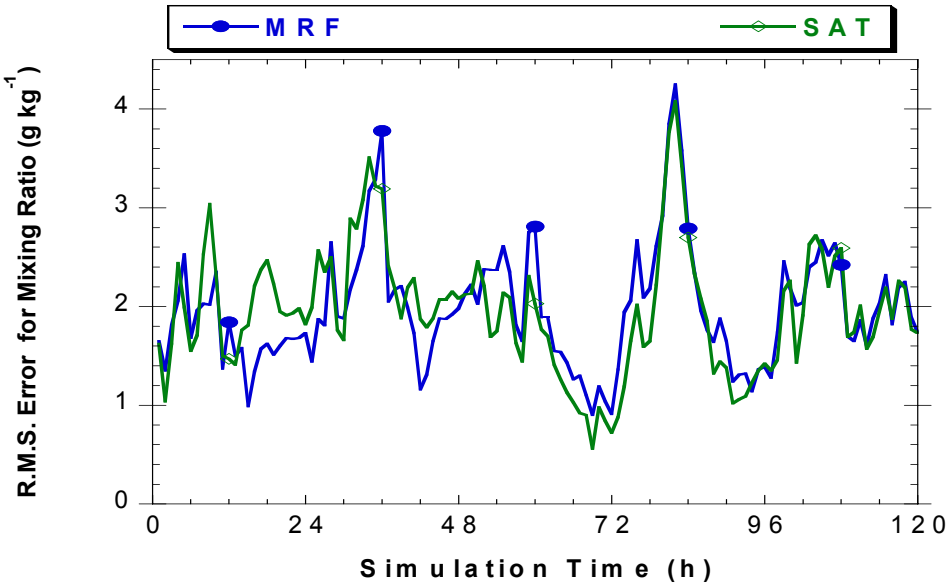
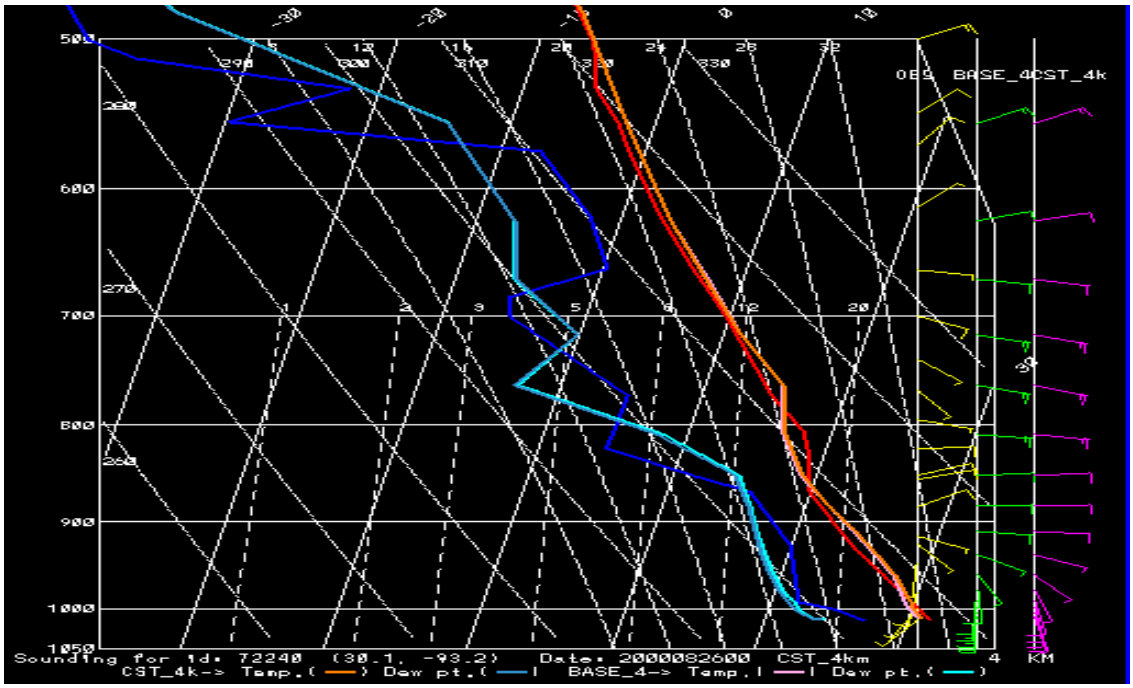
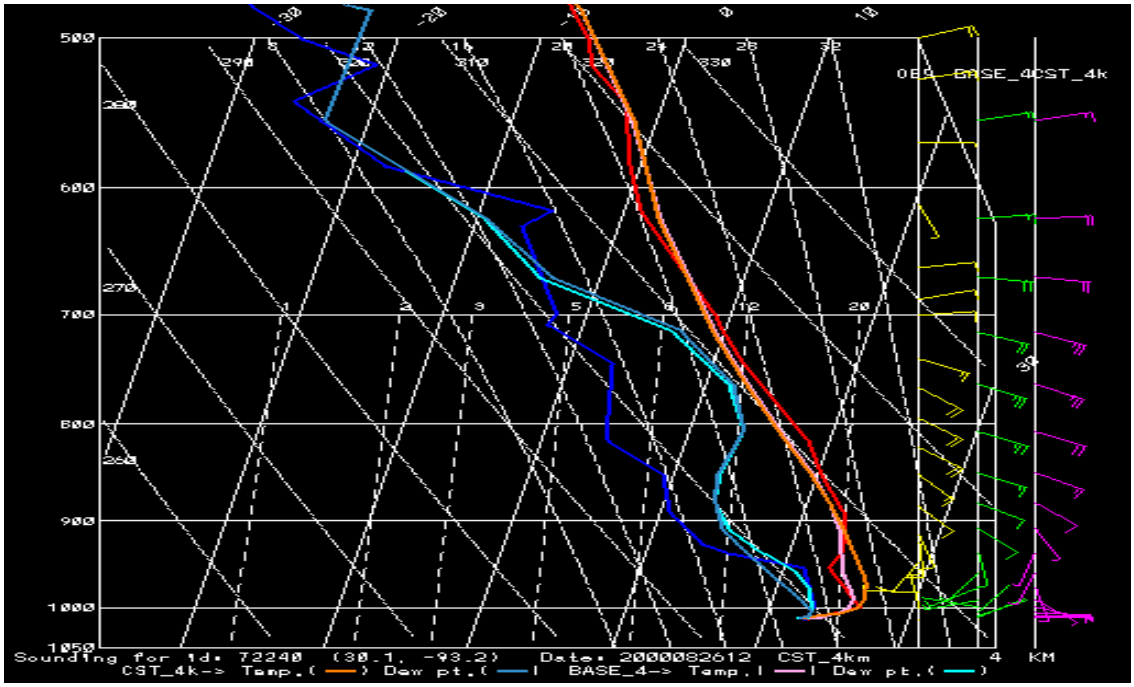


Figure 16b. Temporal variation of near-surface air mixing ratio RMS errors for the "Base" and "Sat" cases using 4-km grids starting at 1200 UTC 23 August 2000.



(a)



(b)

Figure 17. Vertical variation of Temperature, dew point temperature, and horizontal wind vectors for "Obs", "Base", and "Sat" at (a) 00 UTC and (b) 1200 UTC 26 August 2000 for a coastal location in southwest Louisiana.

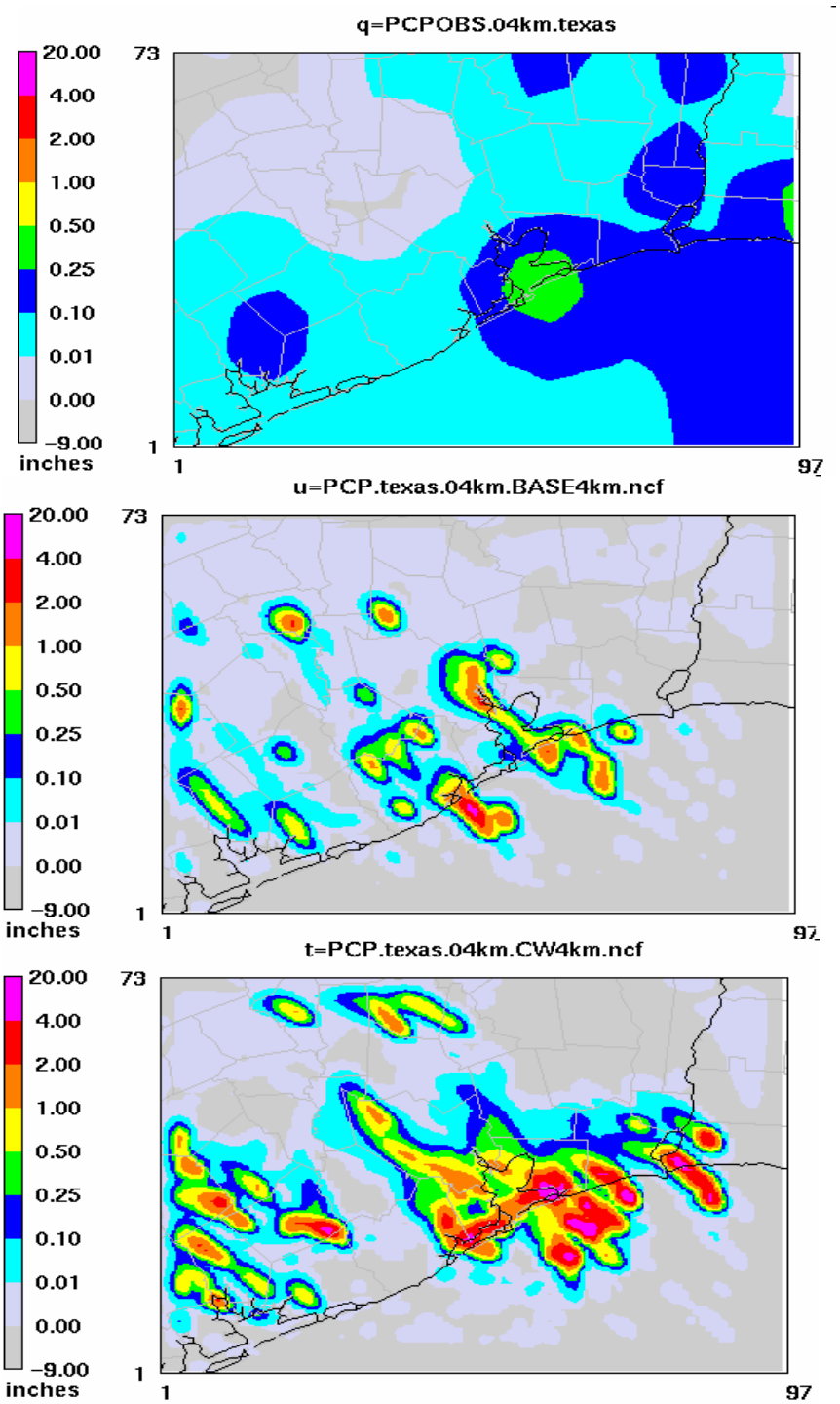


Figure 18a. Accumulated precipitation for the "Obs", "Base" and "Sat" cases, ending at 1200 UTC 24 August 2000 for the 4-km grids.

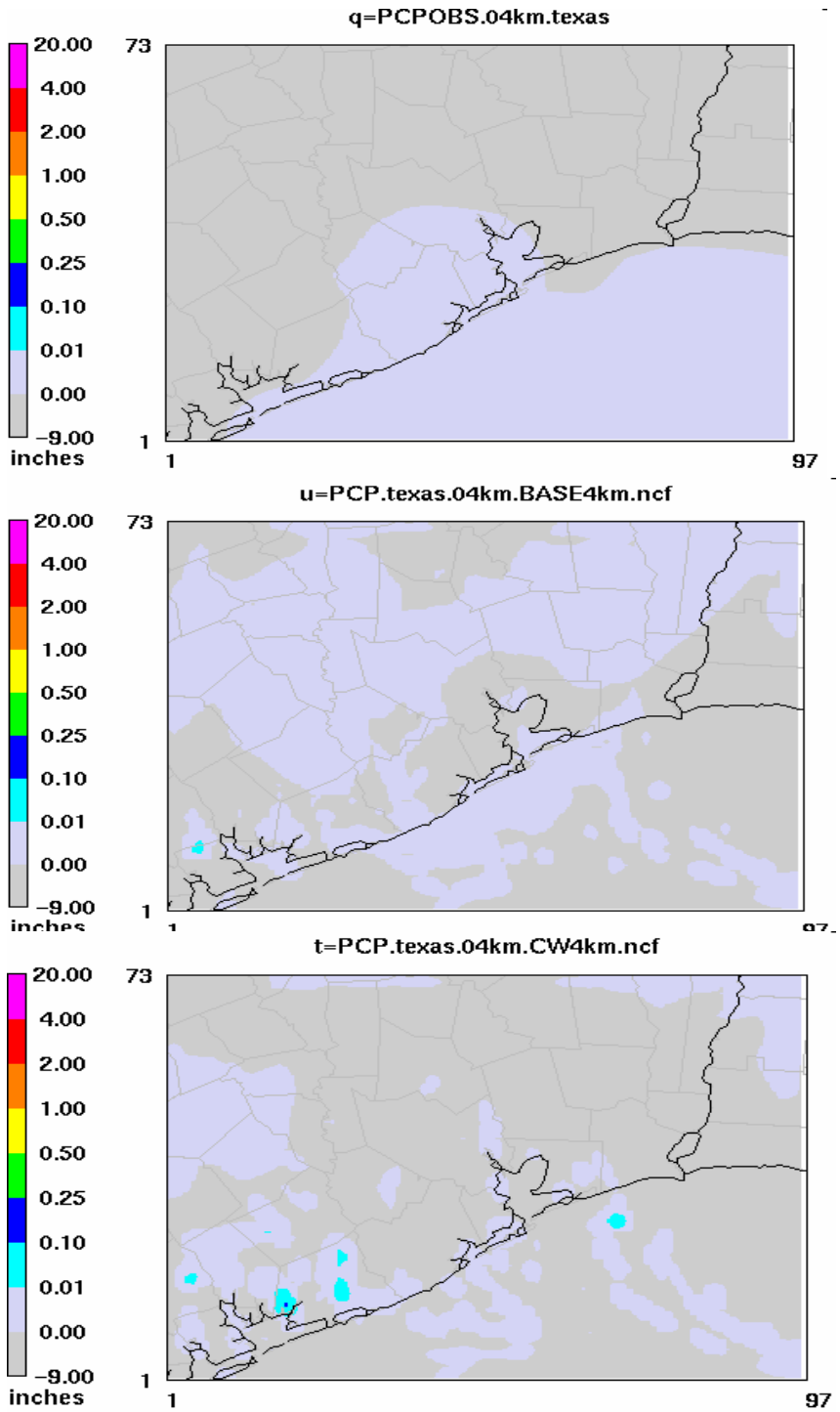


Figure 18b. Accumulated precipitation for the "Obs", "Base" and "Sat" cases, ending at 1200 UTC 28 August 2000 for the 4-km grids.

2.4 Simulate Mesoscale Circulations Using the MM5 (Task 4)

During the second half of the project first year, we completed most of the research in the Tasks 2 and 3. At this stage, we are in a position to develop final MM5 simulations using the best of the configurations according to the results obtained in these two tasks. Early in the second project year, we will generate meteorological fields for input to the MAQSIP-VGR for simulating ozone and aerosol concentrations during an air pollution episode that occurred from 23 August through 2 September 2000.

2.5 Develop Emission Estimates (Task 5)

There are two important issues to be addressed when developing emissions estimates for the MAQSIP-VGR: (1) the SMOKE configurations must be enhanced to handle the variable grids in the MAQSIP-VGR, and (2) offshore point-sources data must be acquired and used to update our emission inventory for the proposed MAQSIP-VGR simulations. The status of these two subtasks during this reporting period (the second half of the first project year) is given below.

2.5.1 Enhancing the SMOKE Configuration

During the first half of the first year, we identified several processing steps that will be changed to support variable grid definitions. The changes required depend on the source category of interest. Some of the major changes needed are (1) correctly translating the latitude-longitude point-source coordinates to the variable-grid cell numbers, (2) correctly translating the latitude-longitude link-source coordinates to the variable-grid cell numbers, and (3) accounting in the variable-grid definitions for the needs of the spatial surrogates. Additional changes are required to allow SMOKE to properly spatially allocate area, nonroad mobile, and on-road mobile nonlink sources. We will address this issue by preparing surrogates that use the variable-grid definition, which will be accomplished by enhancing the Surrogate Tool of SMOKE to read in and use that definition. The resulting surrogates file will use the grid-cell numbers of the variable grid, and SMOKE will process the emissions normally as if the grid were uniform. This approach is the most accurate and requires no changes to SMOKE and no new programs. Other required processing changes are related to biogenic emission estimates, and to configuring plume-rise algorithms for variable grid definitions. We started working on these aspects in the second half of the first year. We refer to the updated SMOKE model as “SMOKE-VGR”.

The development of the SMOKE-VGR was still in progress during the second half of the project’s first year. We anticipate that the SMOKE-VGR will fully be developed and tested during the second project year.

2.5.2 Updating the Emissions Inventory

When the National Emissions Inventory (NEI) 1999 Version 3 becomes available, we will enhance our emission database; this dataset may be available some time in 2004. This will cover updates to area, nonroad, and point sources. For updating mobile sources, we will use MOBILE6 with updated vehicle miles traveled (VMT) data from the Texas Commission on Environmental Quality (TCEQ). Other databases available from TCEQ are a 1999 area/nonroad inventory and a

1997 Galveston Bay shipping inventory. Further, TCEQ has an offshore point- and area-source inventory that we have used in the past; we will contact TCEQ for any updates. We will also use BELD3 land use data to approximate the biogenic emissions (down to 1-km resolution). For the Mexican region, we will use the 1999 BRAVO Mexican inventory. Emissions data for the Outer Continental Shelf in the Gulf of Mexico available from the Minerals Management Service (MMS) will also be included in updating our emissions database. After completing this task, we will use SMOKE-VGR to prepare emissions estimates for use in the MAQSIP-VGR during the second project year.

2.6 Enhance Representation of Cloud Processes in the MAQSIP-VGR (Task 6)

During the first reporting period, we described the adaptation and testing of a cloud mixing algorithm tailored for use with the MAQSIP-VGR.

During the second half of the first year, we implemented this cloud mixing scheme into the MAQSIP-VGR. During the upcoming months, we will test its functionality and evaluate the model results for accuracy. These results will be reported in the next progress report.

2.7 Perform Simulations and Evaluation of the MAQSIP-VGR over the Houston-Galveston Domain (Task 7)

During the first project year, we completed all required evaluations of various ways of developing realistic meteorological inputs. We also identified methodologies to develop a variable-grid version of SMOKE. Development of SMOKE-VGR will be completed during the second project year. Also, during the second project year we plan to develop the variable-grid meteorological and emissions inputs suitable for use in the MAQSIP-VGR. In addition, we will perform a few 10-day simulations (23 August through 2 September) using the MAQSIP-VGR that will focus on the Houston-Galveston region. We will perform two simulations with two different model configurations. In the first configuration, a variable-grid domain over the Houston-Galveston region and offshore will have a high horizontal resolution (~1 km), gradually changing to a coarse resolution of about 12 km at the lateral boundaries of the domain. The second simulation will be for the same domain but will have a very high resolution grid ranging from 400 m to 4 km. These simulations will be completed during the second year.

2.8 Perform Simulations and Evaluation of the MAQSIP-VGR over the Northeast Gulf Domain (Task 8)

After successfully completing the MAQSIP-VGR simulations over the Houston-Galveston region during the second project year, we will perform similar simulations that focus instead on the southern Louisiana region. Details of this work will be presented in upcoming reports. We plan to complete this task during the third (final) year of the project.

Section 3: Conclusion

Various portions of the eight tasks were completed successfully during the second half of the first project year as per the plan and schedule. A comprehensive evaluation of two different atmospheric boundary layer (ABL) schemes (one using a simple MRF scheme, the other using an enhanced physics ETA scheme) indicated that using better ABL physics (i.e., the ETA scheme) in general resulted in marginally improved meteorological simulations using the 36-km grids. However, when used in the 4-km grids, the ETA scheme resulted in excessive and spurious precipitation and hence cloud cover. Since cloud cover has a dramatic influence on ozone photochemistry, we concluded that the MRF scheme should be used to generate meteorological inputs for the MAQSIP-VGR.

Application of our surface data assimilation technique (FASDAS) resulted in dramatic improvements in the meteorological model simulations for the 36-km grids. This result will help us improve our understanding of an air quality model's sensitivity to biogenic emission estimations and differing concentrations of hydrogen peroxide on chemical reactions and resulting pollutant concentrations. The 4-km grids showed a modest improvement with the FASDAS compared to the simulations that did not use the FASDAS. Hence, we will use the FASDAS in generating meteorological inputs for the MAQSIP-VGR.

Use of high-resolution satellite-derived sea surface temperatures (SSTs) in the meteorological model simulations resulted in modest improvements in precipitation simulations compared to using coarse resolution analysis SSTs in the 4-km grids. In view of this positive result, and because diagnostic analysis indicated large differences in various fields between these two simulations, we conclude that we should use satellite-derived SSTs in generating meteorological inputs for the MAQSIP-VGR.

Using the above recommended list of model configurations, we will develop and further evaluate a new set of meteorological inputs that contain all the best features described above. We expect that use of improved meteorological inputs and the highly resolved emission inputs on the variable-resolution grids will lead to improved air quality model simulations. These results will aid us in improving our understanding of the relative contributions of onshore and offshore emissions in dictating air pollution over the coastal regions of the Gulf of Mexico.

In general, our results obtained during the first and second halves of the first year are highly encouraging, and we look forward to disseminating all of our results (including new findings and new methods) to the atmospheric modeling community after developing a few manuscripts.

To perform quality control and analysis of our research results on the VGR domains, we will need to adapt and upgrade a visualization package, the (PAVE). This is necessary because the many other visualization software packages we have tested are not suitable for our research. We are therefore looking into the possibilities for upgrading PAVE for the MAQSIP-VGR. The status of this work will be given in detail in future reports.

Section 4: Publications

Three manuscripts are being written using the research results developed during the first year of this research project. The tentative titles are:

1. Development of a Variable-Grid-Resolution Air Quality Model
2. Development of the Flux-Adjusting Surface Data Assimilation System (FASDAS) for Applications in Mesoscale Models
3. The Effects of Using Satellite-derived Sea Surface Temperatures on Mesoscale Circulations over a Coastal Region and Their Impacts on Air Quality Simulations

We plan to submit these manuscripts for publication in reputable scientific journals.

References

Alapaty, K., N. Seaman, D. Niyogi, and A. Hanna, 2001a: Assimilating Surface Data to Improve the Accuracy of Atmospheric Boundary Layer Simulations. *Journal of Applied Meteorology*, 40, 2068-2082.

Alapaty, K., N. Seaman, D. S. Niyogi, M. Alapaty, G. Hunter, and D. Stauffer, 2001b: Evaluation of surface data assimilation technique using the MM5. *The 11th Penn State/NCAR MM5 Users' workshop, 25-27 June 2001, Boulder, Colorado, USA*.

Alapaty, K., D.S. Niyogi, and M. Alapaty, 2001c: Adjusting soil temperature and moisture using surface observations: Initial results from a single column model. Ninth Conference on Mesoscale Processes, 30 July – 2 August, 2001, Ft. Lauderdale, Florida.

Chen, F., and J. Dudhia, 2001: Coupling an advanced land-surface/hydrology model with the Penn State/NCAR MM5 modeling system. Part I: Model implementation and Sensitivity. Mon. Wea. Rev., 129, 569-585.

Grell, G.A., J. Dudhia, and D.R. Stauffer, 1994. A description of the fifth-generation Penn State/NCAR Mesoscale Model (MM5). NCAR Technical Note NCAR/TN-398+STR.

Nielsen-Gammon, J.W., 2002: Evaluation and Comparison of Preliminary Meteorological Modeling for the August 2000 Houston-Galveston Ozone Episode. Technical report available from the Technical Analysis Division, Texas Natural Resource Conservation Commission, TX.