

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”

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Abstract

This document, the project's first semiannual report, summarizes the research performed from 04/17/2003 through 10/16/2003. Portions of the research in several of the project's eight tasks were completed, and results obtained are briefly presented. We have tested the applicability of two different atmospheric boundary layer schemes for use in air quality model simulations. Preliminary analysis indicates that a scheme that uses sophisticated atmospheric boundary physics resulted in better simulation of atmospheric circulations. We have further developed and tested a new surface data assimilation technique to improve meteorological simulations, which will also result in improved air quality model simulations. Preliminary analysis of results indicates that using the new data assimilation technique results in reduced modeling errors in temperature and moisture. Ingestion of satellite-derived sea surface temperatures into the mesoscale meteorological model led to significant improvements in simulated clouds and precipitation compared to that obtained using traditional analyzed sea surface temperatures. To enhance the capabilities of an emissions processing system so that it can be used with our variable-grid-resolution air quality model, we have identified potential areas for improvements. Also for use in the variable-grid-resolution air quality model, we have tested a cloud module offline for its functionality, and have implemented and tested an efficient horizontal diffusion algorithm within the model.

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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 O₃ 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 six months of project year 1. 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 SO₂ 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 discretizations 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

In the next six-month period, 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 O₃ 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 O₃ 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 portions of the research outline in Section 1. Some of the preliminary results obtained are presented below.

2.1 Develop Modeling Domains and Case Studies (Task 1)

As a starting point for our research, we have developed four domains for use in performing numerical simulations with a meteorological model, the Mesoscale Model Version 5 (MM5)

(Grell et al., 1994), to generate meteorological inputs to the MAQSIP-VGR. These meteorological modeling domains (Figure 1) are configured with different horizontal grid resolutions: 36, 12, and 4 km. In order to specifically study the effects of onshore and offshore emissions on the coastal environments, we have developed two different 4-km grid resolution domains for performing air quality modeling studies, one over the Houston-Galveston region and the other over southern Louisiana.

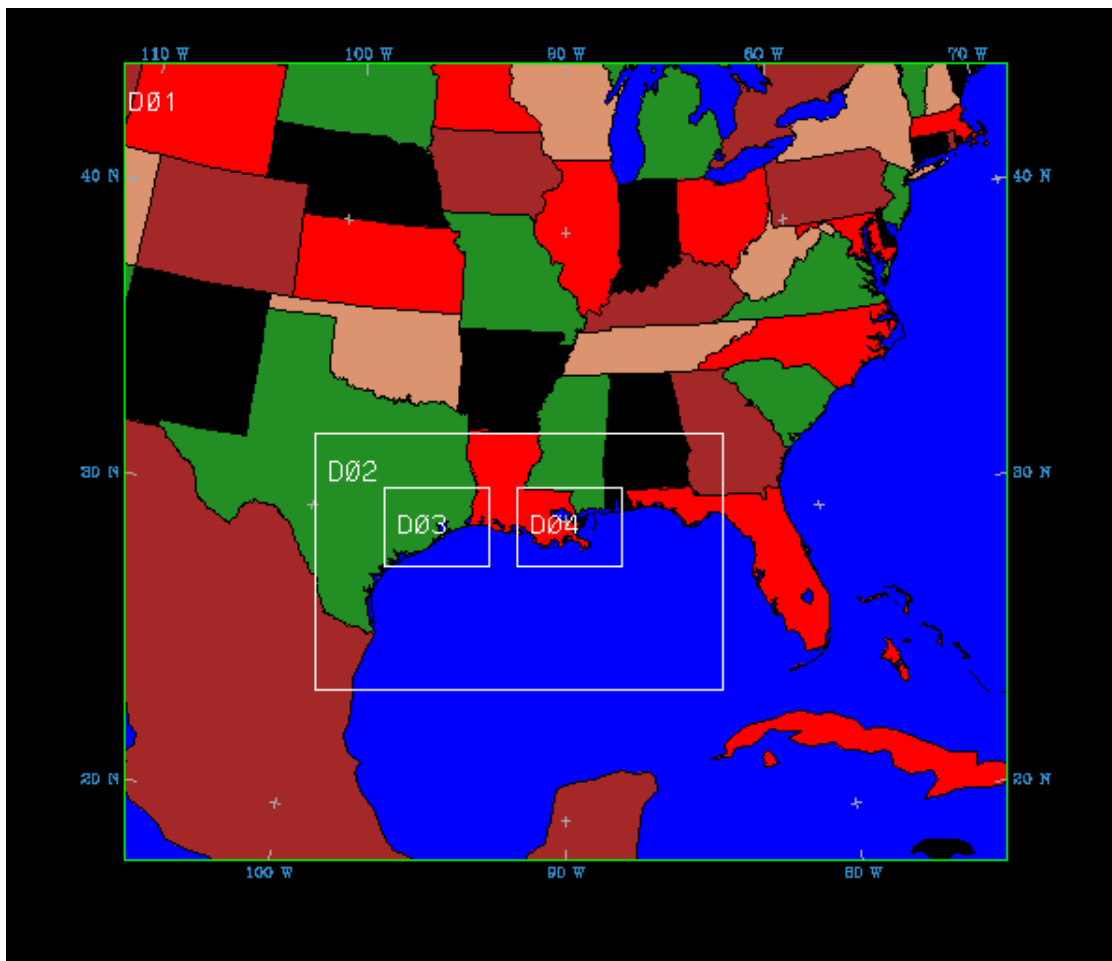


Figure 1. Simulation domains for the MM5 simulations. Domains D01 and D02 use 36- and 12-km grids, respectively, while domains D03 and D04 use 4-km grids located over the Houston-Galveston region and southern Louisiana.

We have selected an initial time period for our numerical simulation case study over the Houston-Galveston region of August 23 to September 2, 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). To provide meteorological inputs to the MAQSIP-VGR, MM5 simulations will be performed for 5.5 days starting from August 23 using the 36-km grid (domain D01). We will use 28 vertical layers to represent atmospheric processes in the

vertical, consistent with the literature (e.g., Neilson-Gammon, 2002). Upon evaluation of results obtained under each of the other tasks, we will perform additional simulations of the MM5 for another 5.5 days starting from August 28.

For the southern Louisiana region, in the second six-month period of the project we will select a time period pertinent for simulating ozone and aerosol concentrations.

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

Although land-sea breeze processes may not be well resolved at the 36-km grid resolution, it is necessary to perform coarse-resolution MM5 simulations to provide lateral boundary conditions to the nested-grid domains delineated in Task 1. At this resolution, we evaluated MM5 simulations that used either an eddy diffusivity-based ABL scheme or a TKE-based ABL scheme. Results obtained from using the eddy diffusivity-based scheme are referred to below as “Base”; those from using the TKE scheme are “Eta.”

We are currently in the process of developing statistical measures (e.g., RMS error, Bias) for several important surface meteorological parameters, and parameters whose accuracy can influence the results from our proposed air quality simulations. We have completed analysis of upper-air soundings simulated by the MM5. Figures 2a through 2d show the observed temperature and dew point temperature soundings (referred to as “Obs”) and modeled soundings obtained from the “Base” and “Eta” cases, for three sites on August 26, 2000; these plots are about three days into the simulations. For the North Platte, Nebraska, site at 0000 UTC (Fig. 2a), the “Base” simulations show cooler temperature profiles ($\sim 1\text{--}3$ K) than both the observations and the “Eta” simulations. For Lake Charles, Louisiana, at 1200 UTC (Fig. 2b), modeling errors are very small with both “Base” and “Eta” and are comparable to each other. For Greensboro, North Carolina, at 0000 (Fig. 2c) and 1200 UTC (Fig. 2d), there are negligible ($\sim \pm 0.5$ K) errors in the simulated temperatures for “Base” and “Eta” when compared to observed soundings. Analysis of several other soundings at various observational times revealed that at 0000 UTC the “Eta” simulations were slightly better than the “Base” ones, while at 1200 UTC the MRF and “Eta” temperature simulations were similar. For water vapor mixing ratio, simulations by the “Eta” seemed to be slightly higher than the measurements (~ 1 g/kg), while “Base” simulations showed slightly lower values (~ -0.5 g/kg) than the observations (figures not shown). Wind profiles show some large errors in the directional component for the coastal regions (e.g., Fig. 2b) in both the “Base” and “Eta” simulations, particularly in the ABL, while aloft wind speed and direction are very close to the observations for both “Base” and “Eta”. As an example, we show the horizontal wind vectors simulated by the “Base” and “Eta” (Figs. 3a and 3b), which reveal differences in the wind direction and speed over the coastal regions of the Gulf of Mexico.

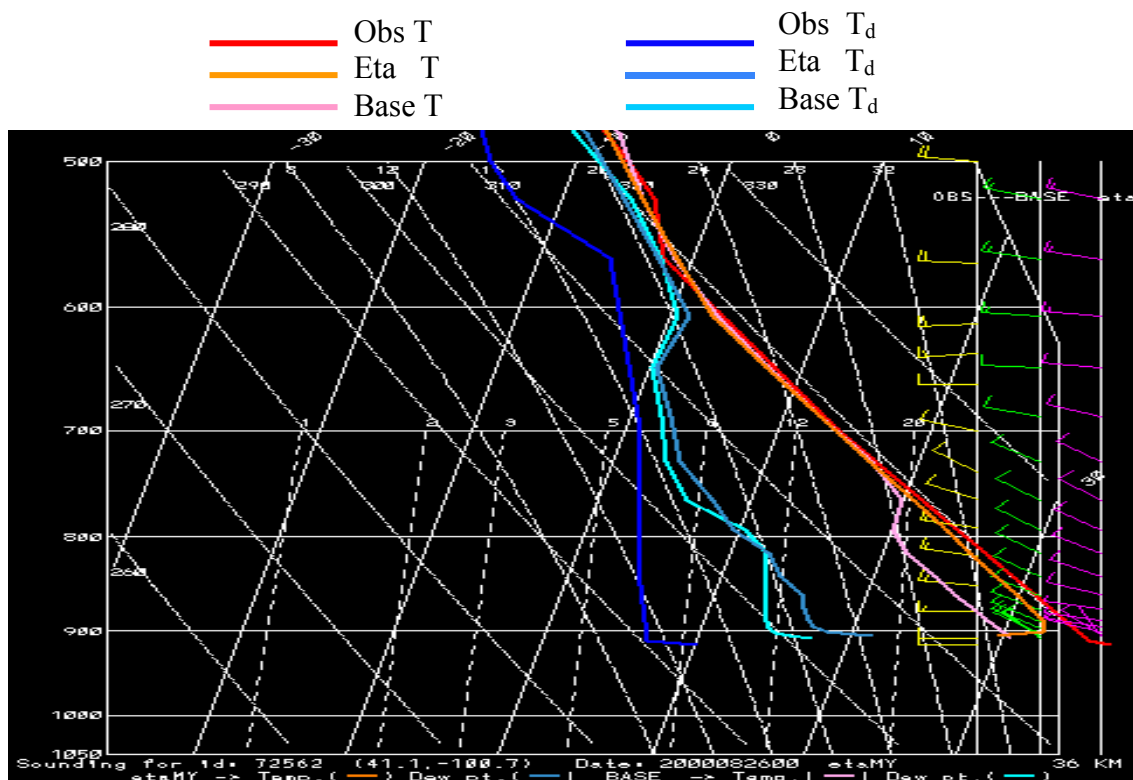


Figure 2a. Vertical variation of observed and simulated temperature and dew point temperature soundings for North Platte, Nebraska, at 0000 UTC on August 26, 2000.

Legend for Wind Barbs:

Yellow – “Obs”
 Green – “Base”
 Magenta – “Eta”

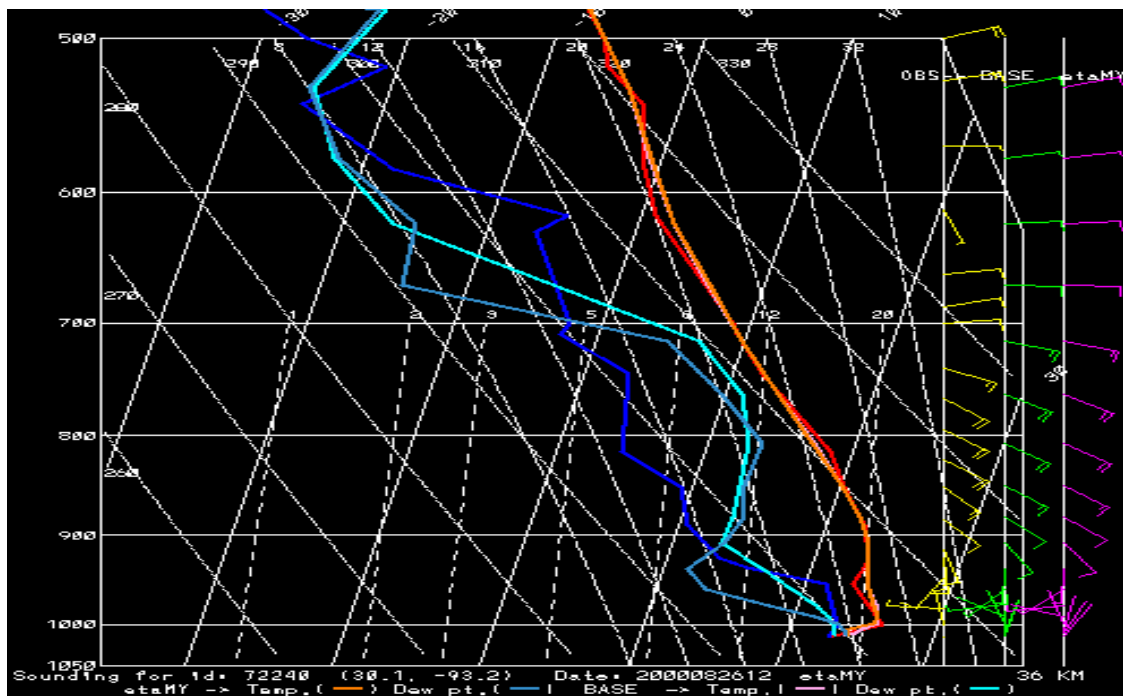


Figure 2b. Vertical variation of observed and simulated temperature and dew point temperature soundings for Lake Charles, Louisiana, at 1200 UTC on August 26, 2000.

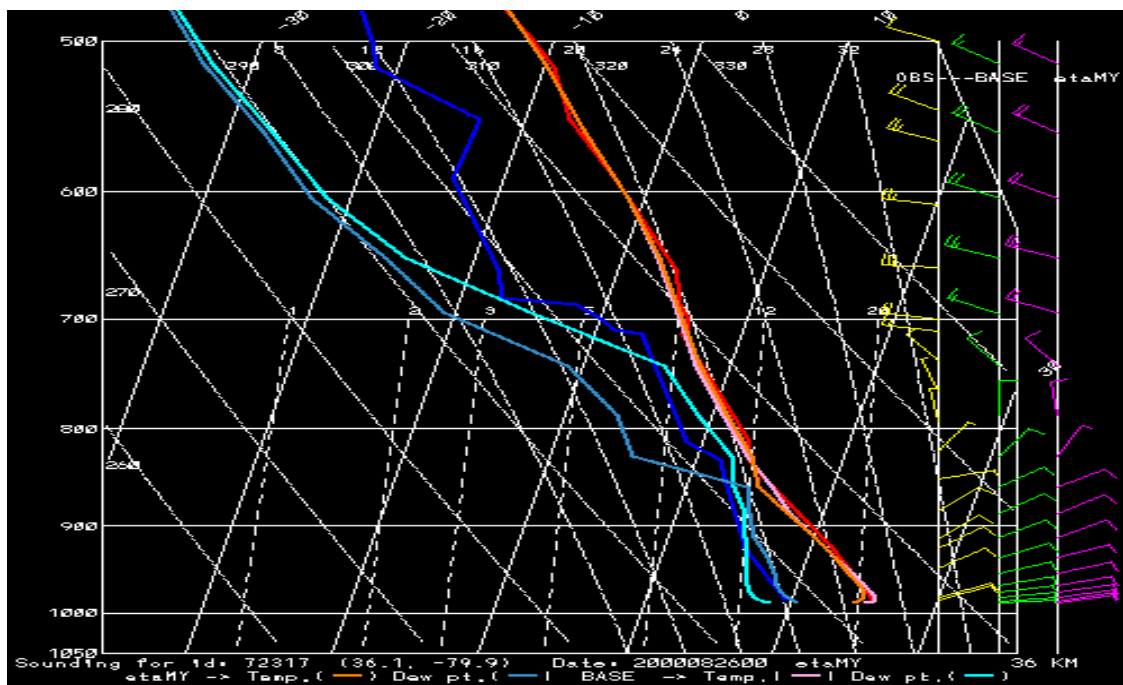


Figure 2c. Vertical variation of observed and simulated temperature and dew point temperature soundings for Greensboro, North Carolina at 0000 UTC on August 26, 2000.

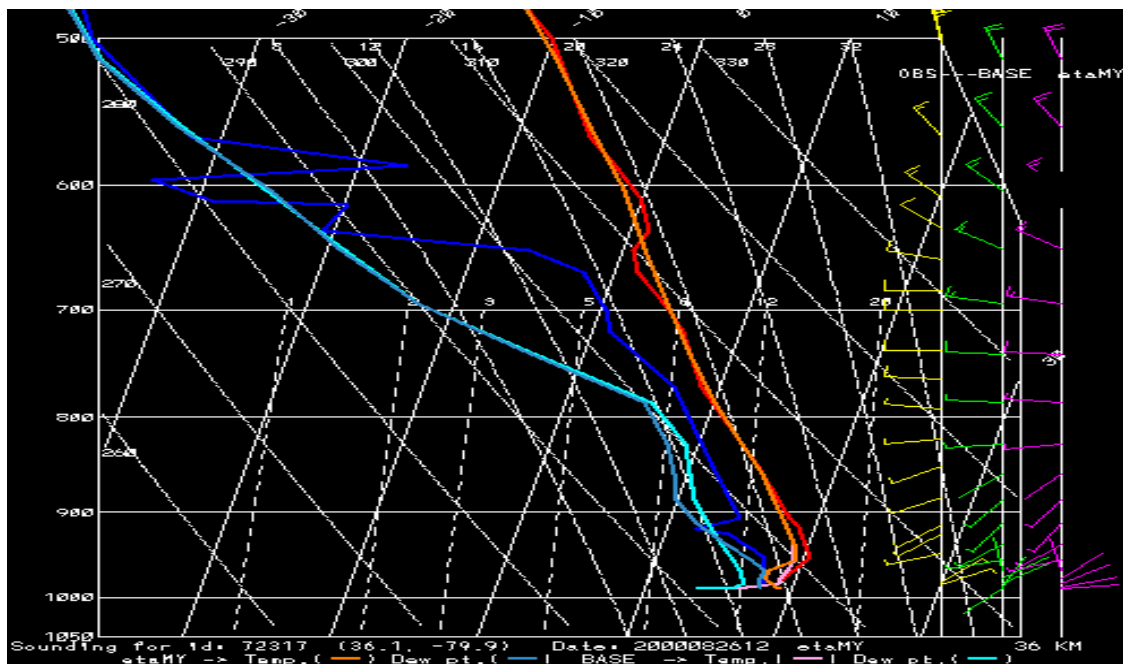


Figure 2d. Vertical variation of observed and simulated temperature and dew point temperature soundings for Greensboro, North Carolina at 1200 UTC on August 26, 2000.

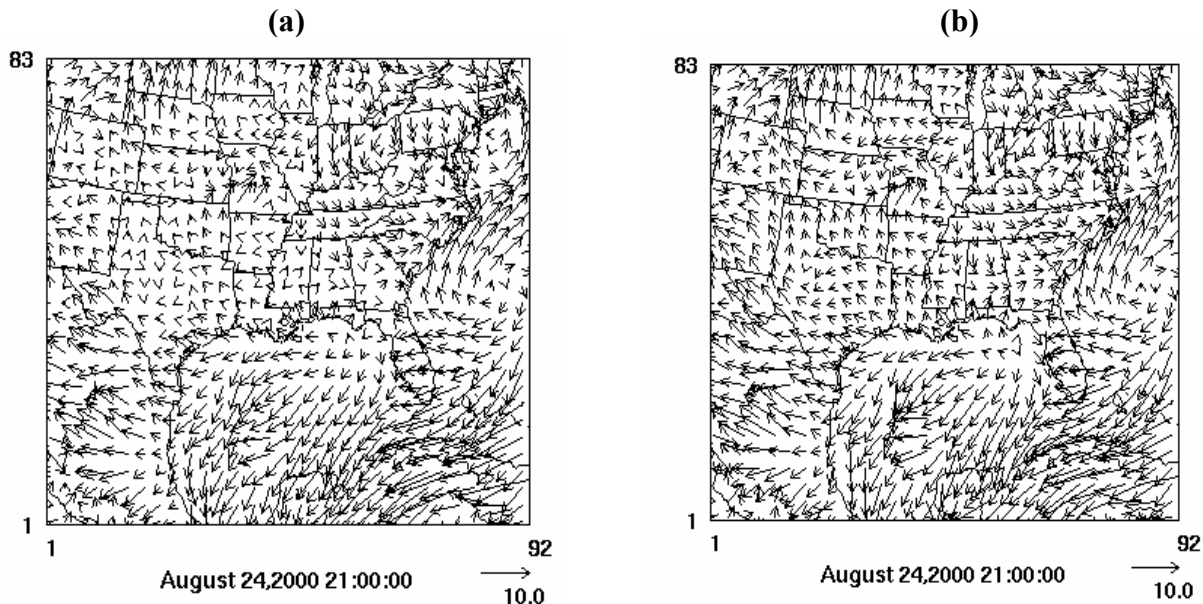


Figure 3. MM5 simulated horizontal wind vectors at 2100 UTC August 24, 2000, from (a) “Base” and (b) “Eta” simulations using the 36-km grids.

We are in the process of acquiring more observations and performing further evaluations of these simulations. During the next semiannual period, we will perform MM5 simulations using the 12- and 4-km grids focusing on the Houston-Galveston region and southern Louisiana region. We will also acquire radar data for evaluating ABL depths over the coastal and inland regions, GOES-based remotely sensed data for evaluating cloud fractions, and Stage IV precipitation data to evaluate simulated precipitation amounts in the “Base” and “Eta” cases. Our analysis indicated that there are differences in simulated cloud cover between the “Base” and “Eta” cases, and also in the simulated total precipitation (Figure 4). Over the Houston-Galveston region, the “Base” simulations may be indicating higher precipitation rates than those in the “Eta”. Since the “Base” and “Eta” cases used a coarse grid resolution, it is normal to expect underprediction of precipitation amounts. After completing high-resolution simulations (i.e., 4-km grids), we will compare model simulations with the Stage IV RADAR precipitation estimates available from NCDC.

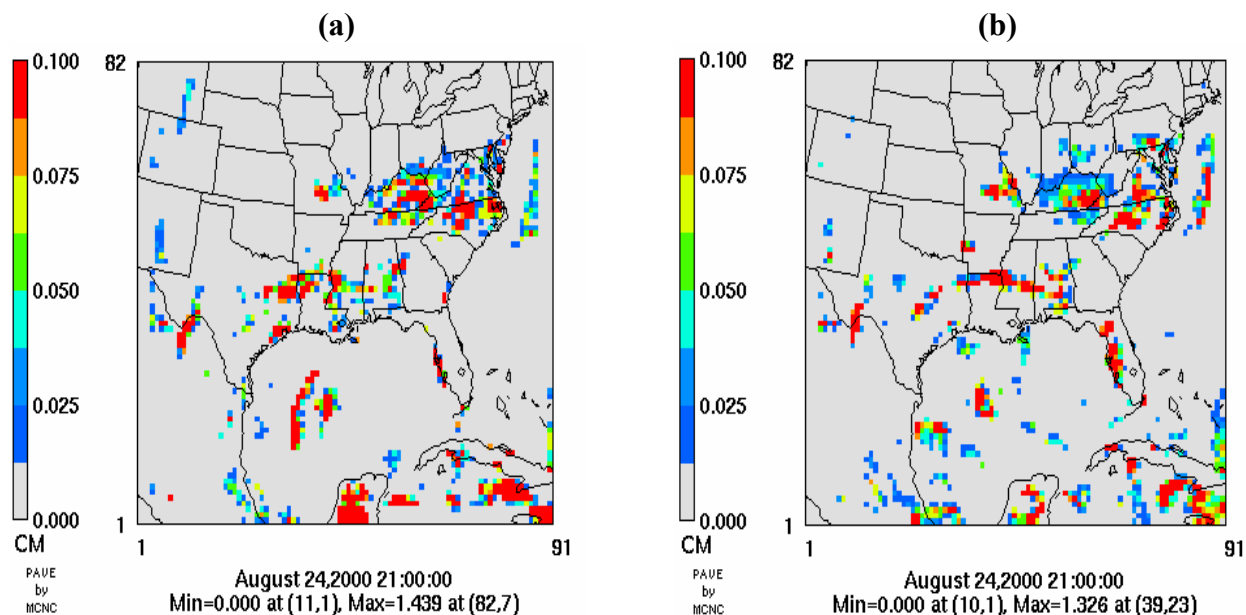


Figure 4. MM5 simulated total precipitation (cm/h) at 2100 UTC August 24, 2000, from the (a) “Base” and (b) “Eta” simulations using the 36-km grids.

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.

For this project, we have 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 to compare with the “Base” simulations described in Section 2.2. One of the reasons for using the MRF scheme as a default ABL scheme in the MM5 simulations is the fact that it is most widely used scheme. However, in the future, we will implement the FASDAS into the TKE scheme (Eta) used in the simulations described in the Section 2.2.

We have performed some preliminary analysis and evaluation of the results obtained using FASDAS technique in the MM5. The MM5 simulations using the MRF scheme discussed in Section 2.2 (which was referred to as “Base”) are used here as a benchmark to evaluate the MM5 results obtained using the FASDAS.

Figure 5 shows the number of hourly surface observations used as a function of time to develop several statistical indices to evaluate MM5 model simulations using and without using the FASDAS. Each of observational sites is paired with the corresponding grid cell in the modeled

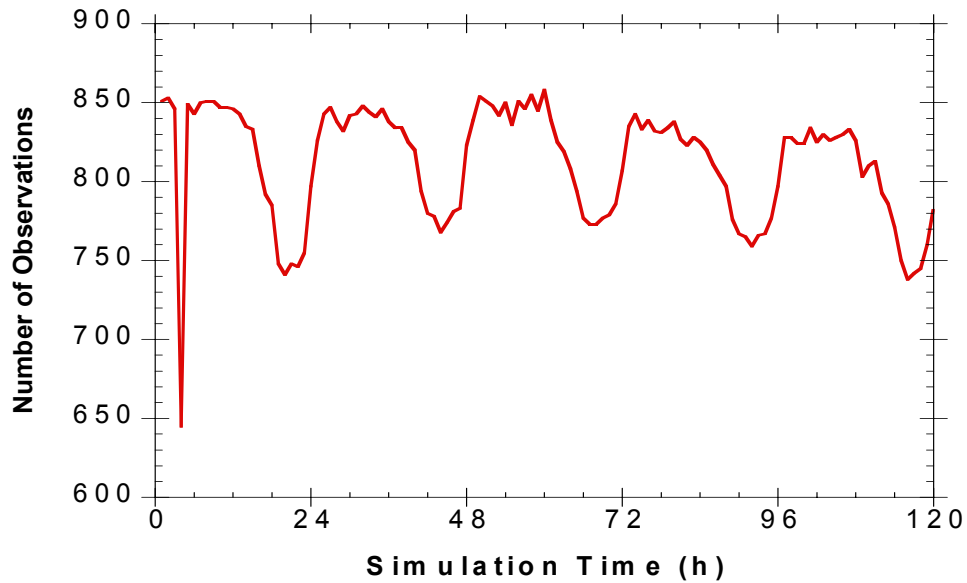


Figure 5. Temporal variability in the number of available surface observations used in developing statistical indices. Zero on the x-axis corresponds to 1200 UTC 23 August 2000.

domain for preparing statistics. Simulated temperature, mixing ratio, and winds for these representative grid cells are then interpolated from the model’s lowest-level altitude to the respective measurement heights to facilitate direct intercomparison. In Figures 6 through 12, the

observations are referred to as “Obs”; the model results obtained using the MRF scheme, which did not assimilate any surface data, are “Base”; and the simulations that used MRF along with the FASDAS are “Fasdas.” The quantity (M–O) is used in preparing many statistics (e.g., Bias shown in Fig. 7), where 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.

Figure 6 shows the temporal variation of near-surface temperature (K). It is clear that the application of the FASDAS led to improved temperature simulations compared to the “Base” simulations. Improvement is evident in the temporal variation of bias for near-surface temperature (K) (Figure 7). This result has favorable implications for air quality modeling because it could lead to improved representation of biogenic emission estimates over vegetated regions. Figure 8 shows the temporal variation of bias for near-surface water vapor mixing ratio (g/kg). When interpreting this figure, it is important to understand that the observations are available at 2 m AGL while the modeled values for water vapor mixing ratio were available at about 18 m AGL. Since there is no robust method for interpolating mixing ratio to the observational height of 2 m, we have used modeled values for the lowest model layer. Hence, the positive bias present in the “Fasdas” results at night may not necessarily indicate overprediction, since dew formation that may exist near the surface can lead to drier layers near the surface versus aloft. In general, model simulations for the “Fasdas” case compare favorably with observations, indicating overall improvements in the simulations compared with “Base.” This result could also have a positive impact on air quality model simulations through improved representation of H₂O₂ concentrations.

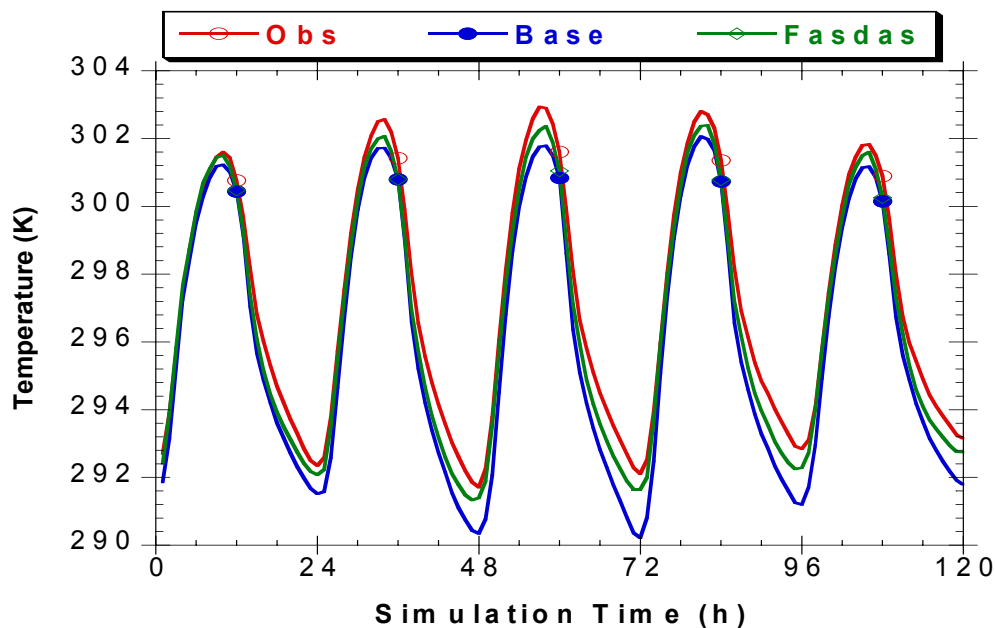


Figure 6. Temporal variation of near-surface air temperature averaged over all of the measurements and corresponding modeled values, starting at 1200 UTC 23 August 2000.

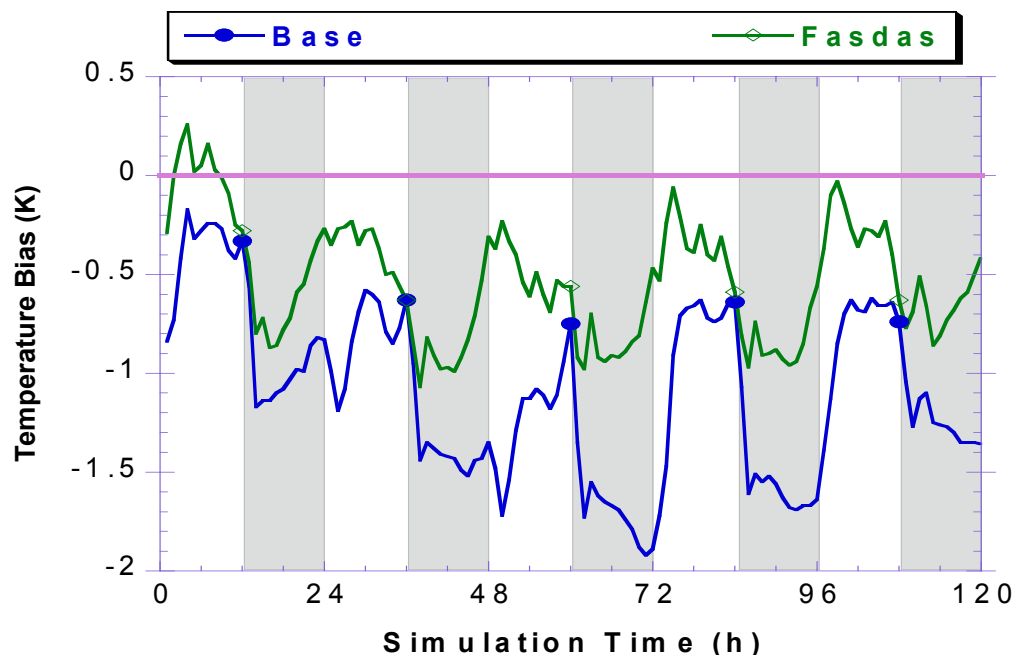


Figure 7. Temporal variation of bias in the averaged near-surface air temperature for the “Base” and “Fasdas” cases, starting at 1200 UTC 23 August 2000.

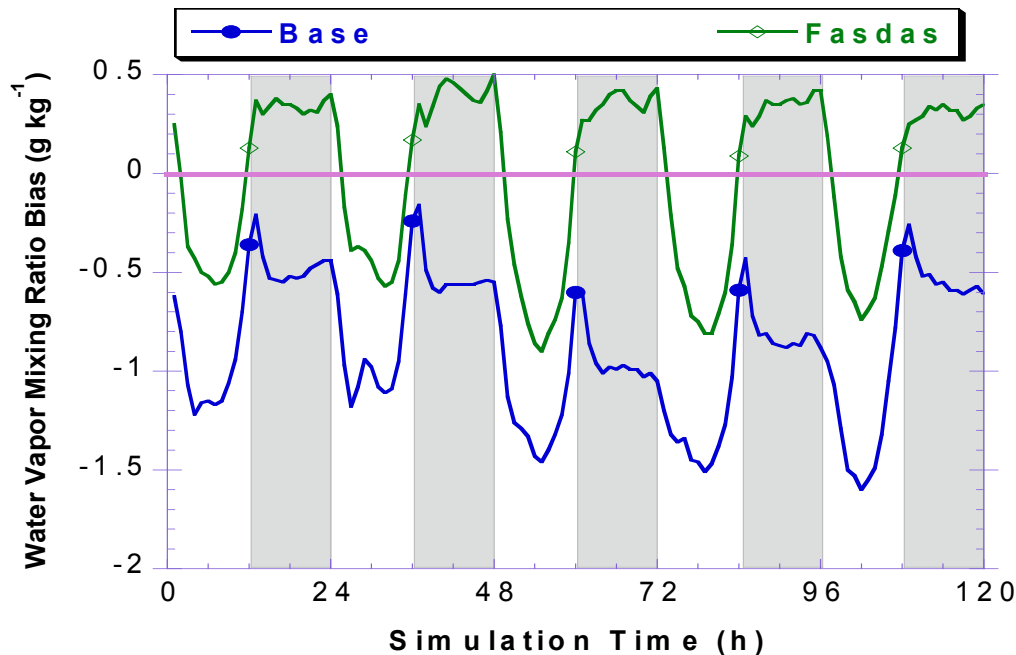


Figure 8. Temporal variation of bias in the averaged near-surface air water vapor mixing ratio for the “Base” and “Fasdas” cases, starting at 1200 UTC 23 August 2000.

Figures 9 through 12, for four different geographic locations and dates, show the vertical variation in observed temperatures and dew point temperatures together with the corresponding modeled profiles obtained from the “Base” and “Fasdas” cases. Generally, there is improvement in the simulation of vertical soundings when FASDAS is used. Also, the differences between “Base” and “Fasdas” for wind speed and direction are negligible. In this case study, the FASDAS technique reduced errors in the modeled temperature and water vapor mixing ratio in the lowest layers and aloft. We will continue further analysis and will include results in future reports.

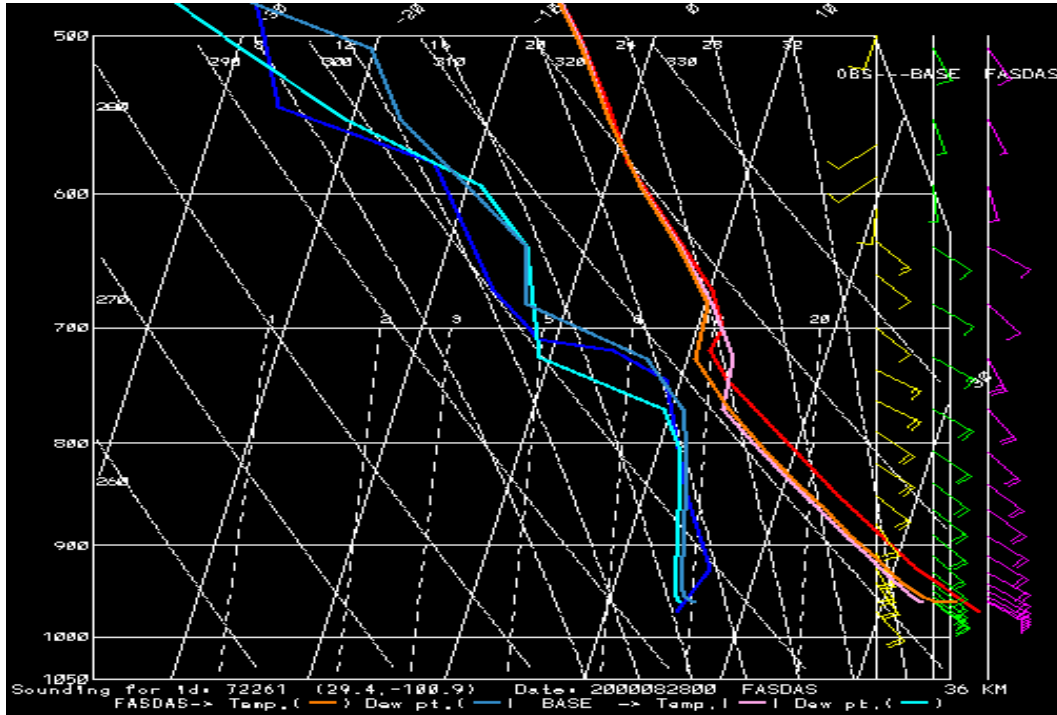


Figure 9. Vertical variation in temperature and dew point temperature from observations and the “Base” and “Fasdas” cases at 0000 UTC 28 August 2000 for Del Rio, TX.

Legend for Sounding Plots:

Wind Barbs: Yellow – “Obs”
 Green – “Base”
 Magenta – “Fasdas”

—	Obs	T	—	Obs	T _d
—	Fasdas	T	—	Fasdas	T _d
—	Base	T	—	Base	T _d

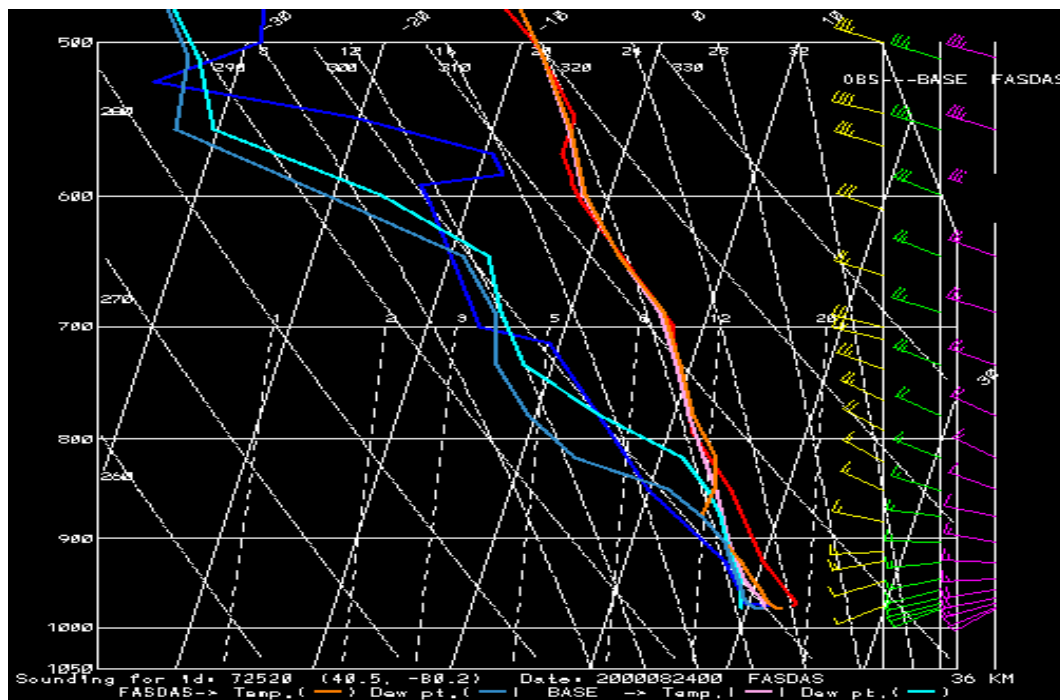


Figure 10. Vertical variation in temperature and dew point temperature from observations and the “Base” and “Fasdas” cases at 0000 UTC 24 August 2000 for Pittsburgh, PA.

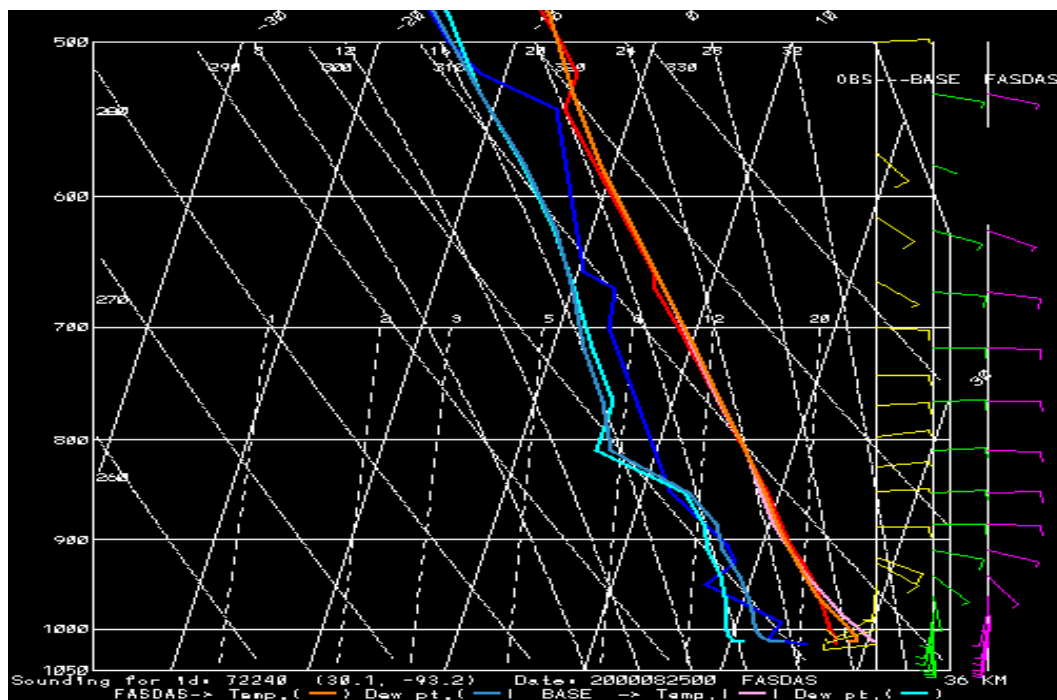


Figure 11. Vertical variation in temperature and dew point temperature from observations and the “Base” and “Fasdas” cases at 0000 UTC 25 August 2000 for Lake Charles, Louisiana.

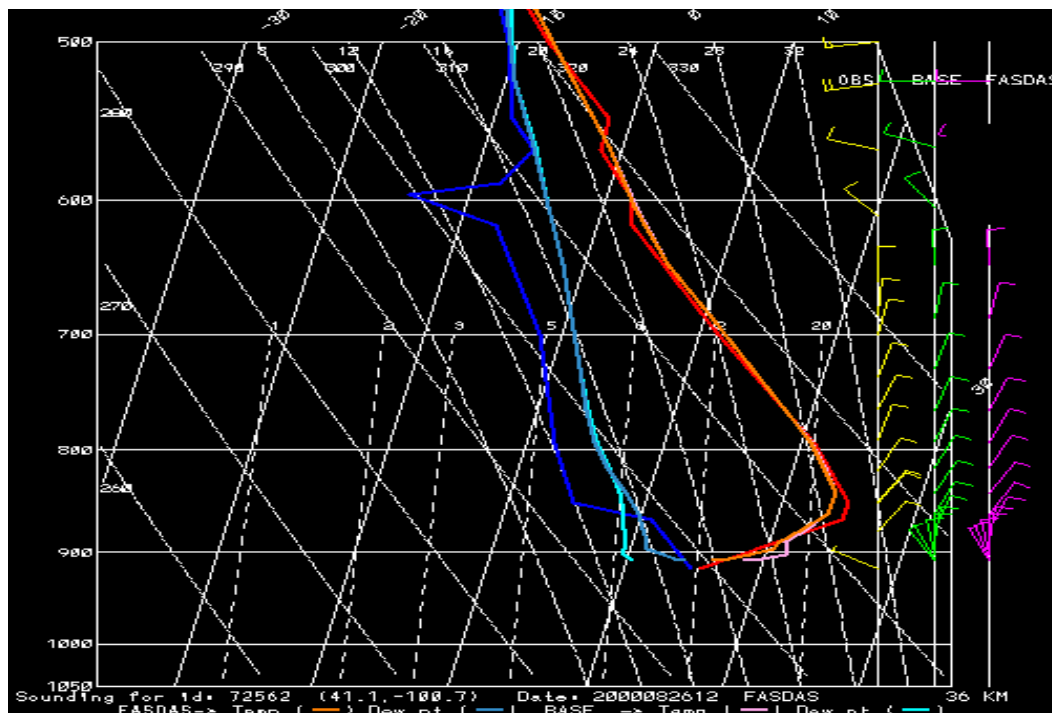


Figure 12. Vertical variation in temperature and dew point temperature from observations and the “Base” and “Fasdas” cases at 0000 UTC 26 August 2000 for North Platte, Nebraska.

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. This leads to a bulk representation of SSTs that could lead to some modeling errors, particularly over the coastal regions such as Houston-Galveston region.

We acquired remotely sensed SSTs at 4x4 km resolution archived by NOAA for a small region east of the Houston-Galveston region. 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 preprocessing 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 (Domain D03 in Figure 1) 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. In the future, we will acquire remotely-sensed SSTs suitable for the domains D01 (36 km grids) and D02 (12 km grids) and repeat these simulations for the D01 and D02 domains and finally The D03 as well as D04 domains (see Fig. 1).

Figure 13a shows the spatial distribution of SSTs obtained from processing the traditional NCEP analysis, while Figure 13b shows the SST distribution obtained using NOAA's satellite measurements. There is a large difference in the magnitudes and spatial distributions of SST gradients for the period considered in this study. These two differing SST datasets were used to perform the MM5 simulations for the 4-km Domain D03 to investigate how using different SSTs affects the model simulations. Some preliminary analysis results are presented here. Results obtained from using the analyzed SSTs and satellite-derived SSTs are referred to in the text as "Base" and "Sat," respectively.

Since large differences in the SSTs were present, we used an eastern subregion of the Houston-Galveston domain (highlighted in the Figure 14) for analyzing average properties of different variables simulated by the MM5. The main reason to consider this subregion is that during the daytime easterly winds dominate the general flow pattern where winds from the Gulf seeps into the H-G region. Thus, usage of differing SSTs should have an impact on the mesoscale dynamics and circulation pattern. Figure 15a shows the temporal variation in the area-averaged surface latent heat flux for the subregion for the "Base" and "Sat" cases. The latent heat fluxes are about 100% higher in the "Sat" case than in "Base." Figure 15b shows the temporal variation in the area-averaged depth of the boundary layer. Warmer sea surface temperatures resulted in an increased ABL depth for the "Sat" case. In future months, we will also examine the mixing intensity and atmospheric stability over these marine environments, as these can play an important role in air quality model simulations through (1) diluting air pollutants in the ABL and (2) recirculating pollutants over the coastal regions through land-sea breezes.

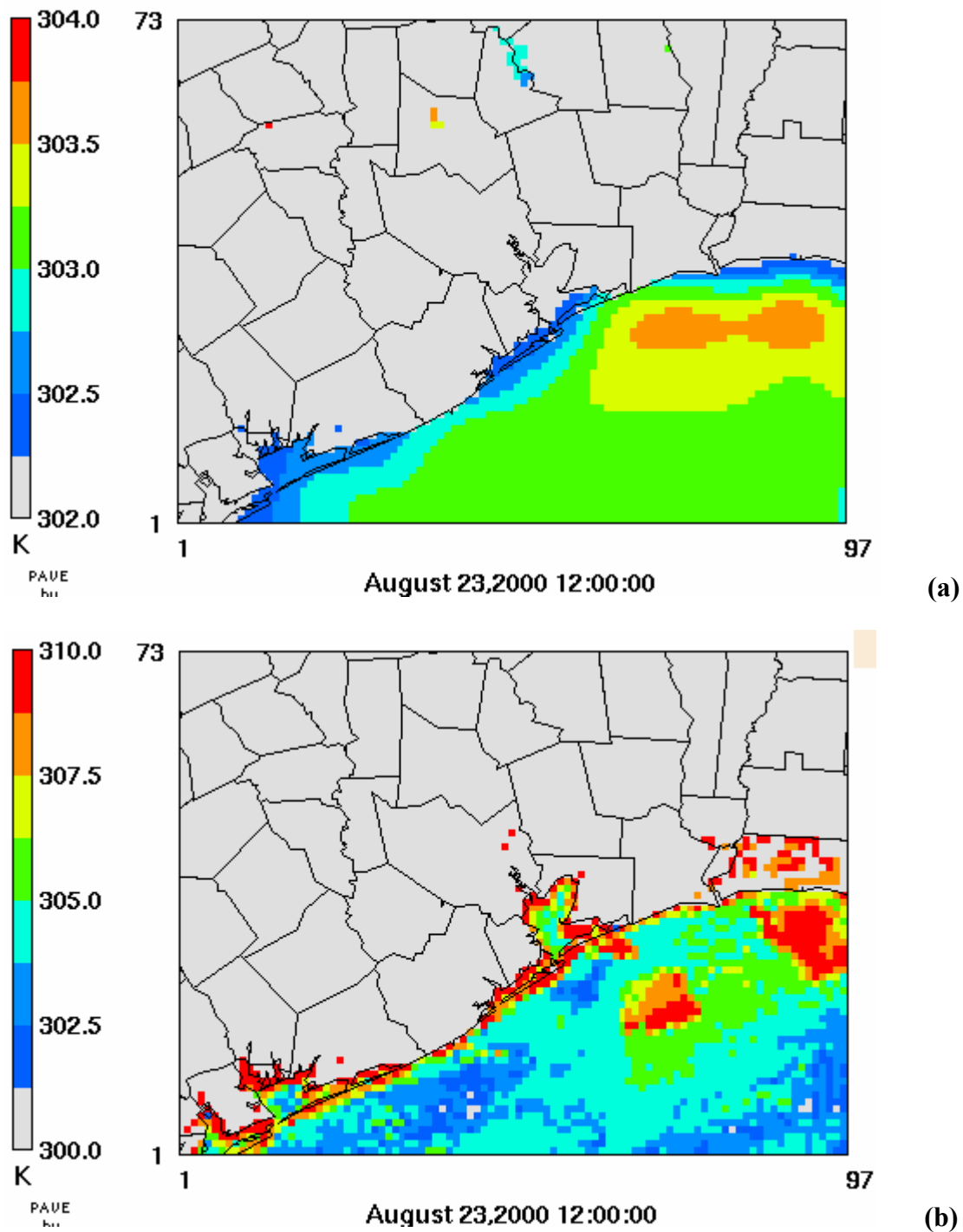


Figure 13. Spatial distribution of sea surface temperatures in Domain D03 obtained from (a) the traditional NCEP analysis and (b) NOAA's satellite-derived measurements, at 1200 UTC 23 August 2000. Note the difference in the scale ranges.

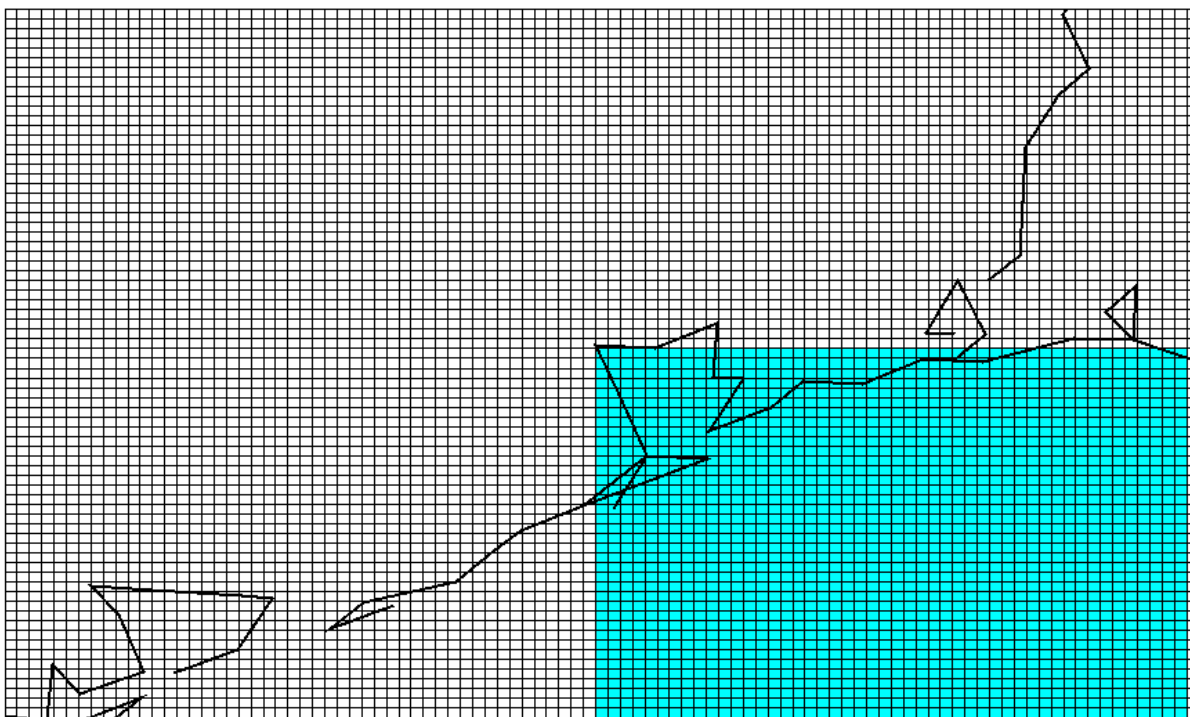
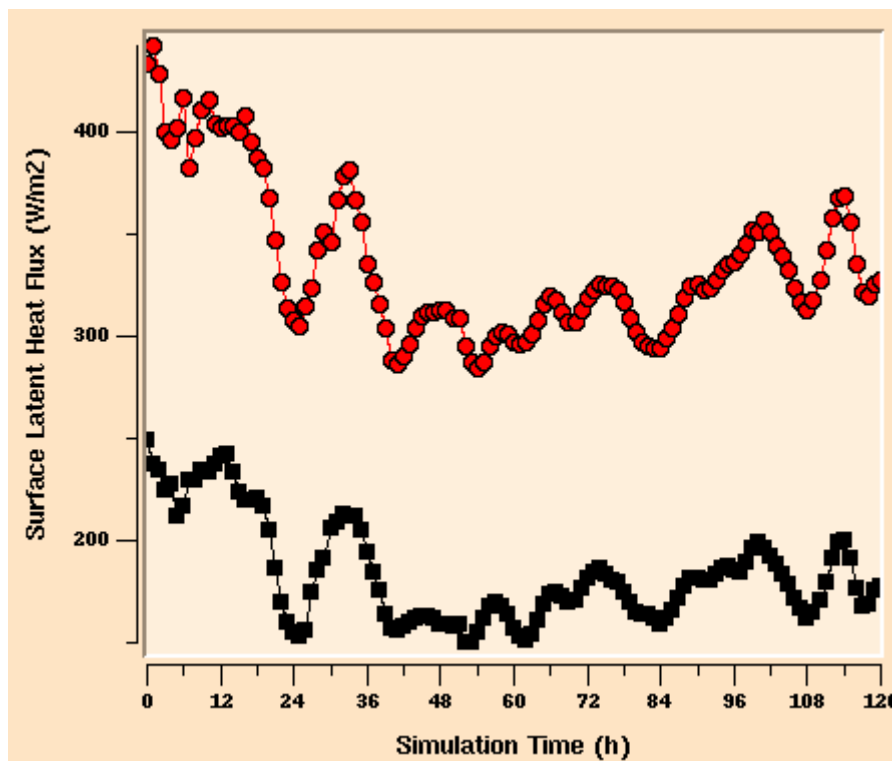
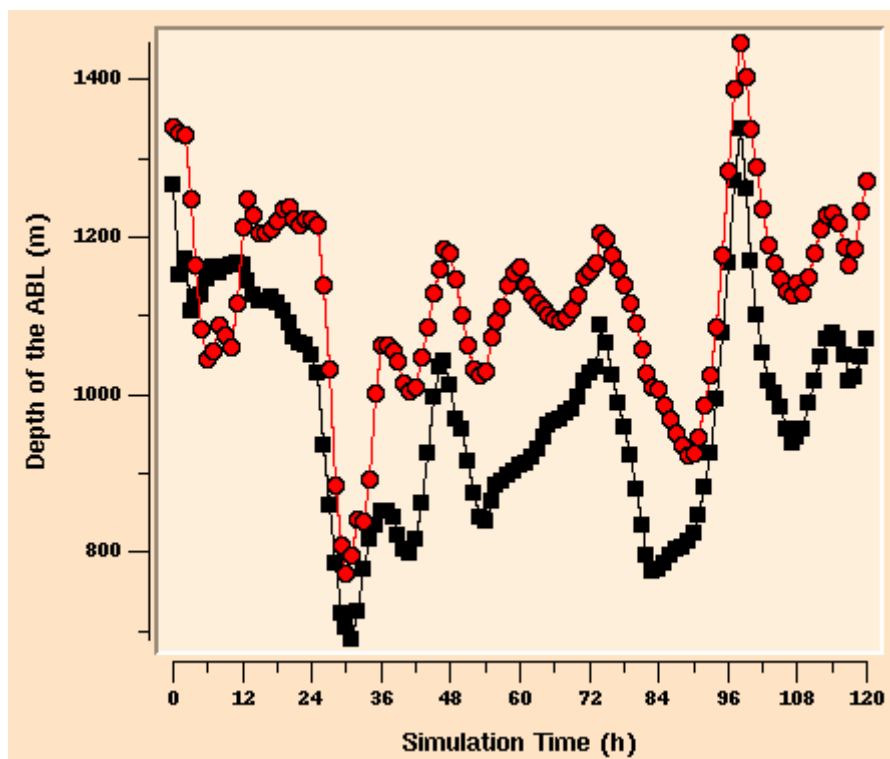


Figure 14. Portion of Gulf of Mexico considered (highlighted grid cells) in developing area-averaged meteorological parameters for analysis and intercomparison.



(a)



(b)

Figure 15. Area-averaged (a) surface latent heat fluxes and (b) depth of the ABL, over the Figure 14 subregion of the Gulf of Mexico. Black: “Base” – Red: “Sat”

Figure 16a shows radar imagery at 2100 UTC 24 August 2000 obtained from the study of Neilson-Gammon (2002); it indicates regions of light (cool colors) and heavy (hot colors) precipitation. Because we used a 4-km resolution, convection and associated precipitation may be sufficiently resolved by the explicit cloud scheme used in the MM5 simulations. We compared the shortwave radiation reaching the ground in the “Base” and “Sat” cases (Figs. 16b and 16c). Once clouds form, they may not lead to precipitation in the model. However, it affects the amount of shortwave radiation reaching the surface. Thus, shortwave radiation reaching the surface can be used as a surrogate for cloud activity. Closer examination of Figs. 16a, 16b, and 16c shows greater similarity between the radar measurements and the “Sat” case, while “Base” has highly underpredicted cloud amounts. Observed precipitation over Galveston Bay and north and east of the Houston-Galveston region is better simulated by the locations of clouds in the “Sat” case. Figures 17a and 17b show the total accumulated precipitation for the hour ending at 2100 UTC 24 August 2000 for the “Base” and “Sat” cases. Qualitative comparison of images in Figs. 16 and 17 suggest that the “Sat” case models precipitation far better than the “Base” case does. This demonstrates the necessity of using realistic sea surface temperatures in meteorological modeling.

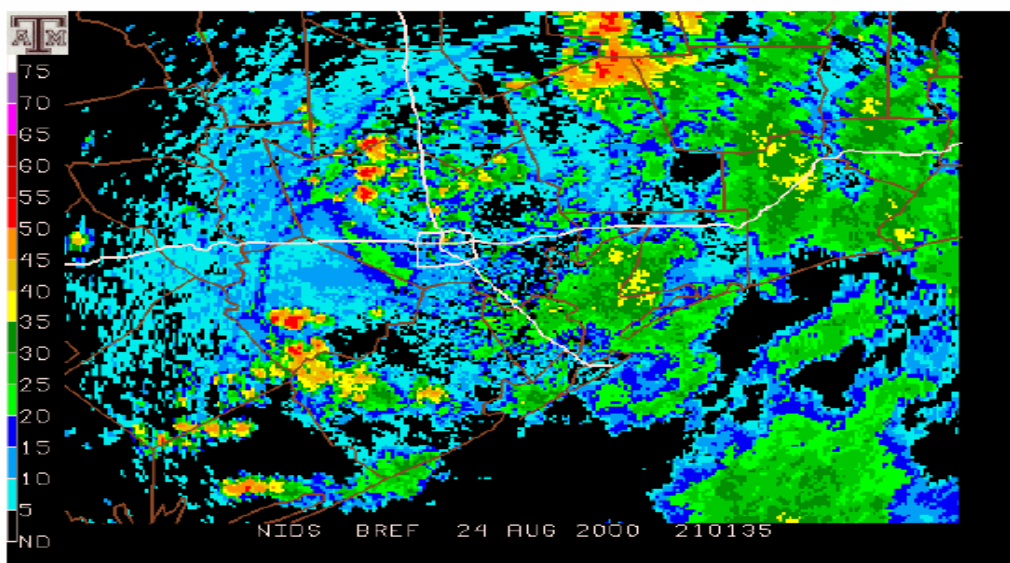
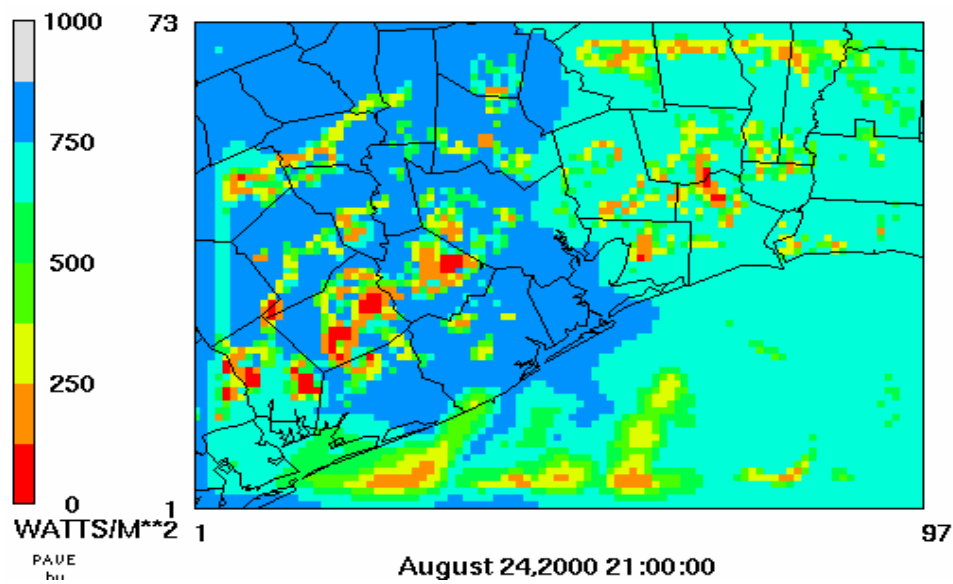
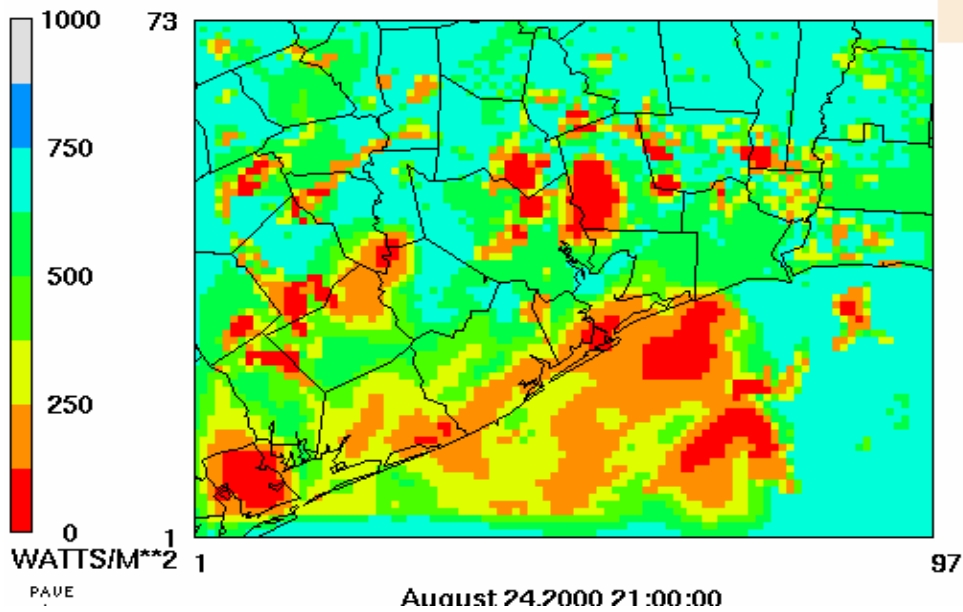


Figure 16a. Radar imagery of reflectivity showing intensity of precipitation at 2100 UTC 24 August 2000, obtained from a study by Neilson-Gammon (2002).

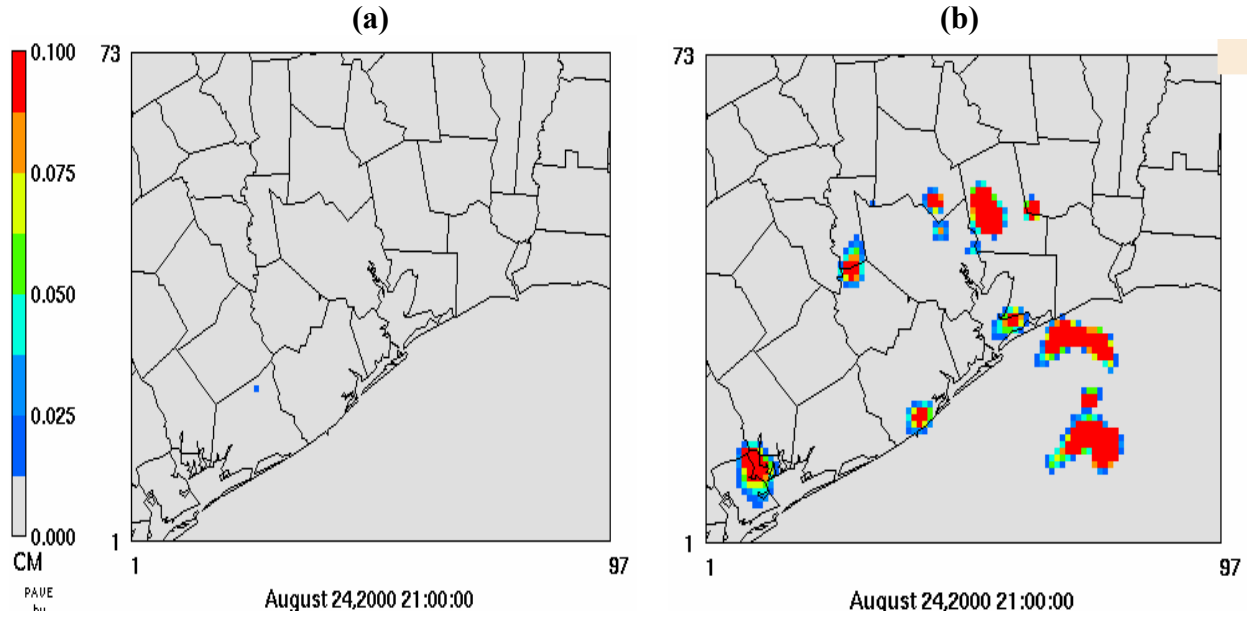


(b)



(c)

Figures 16b, 16c. Modeled shortwave radiation reaching the surface (W/m^2) at 2100 UTC 24 August 2000 for the (b) "Base" and (c) "Sat" cases.



Figures 17. Modeled total precipitation (cm/h) for an hour ending at 2100 UTC 24 August 2000 for the (a) “Base” and (b) “Sat” cases.

Using realistic SSTs also significantly affects the modeling of the land-sea breeze; this is clearly evident in the moisture distribution near the surface and aloft. Figures 18a and 18b show the model’s lowest-level moisture and its vector flux on August 25 for the “Base” and “Sat” cases, indicating dramatic effects on the precipitation events present at that time. We will continue analyzing these results and report our findings in the near future.

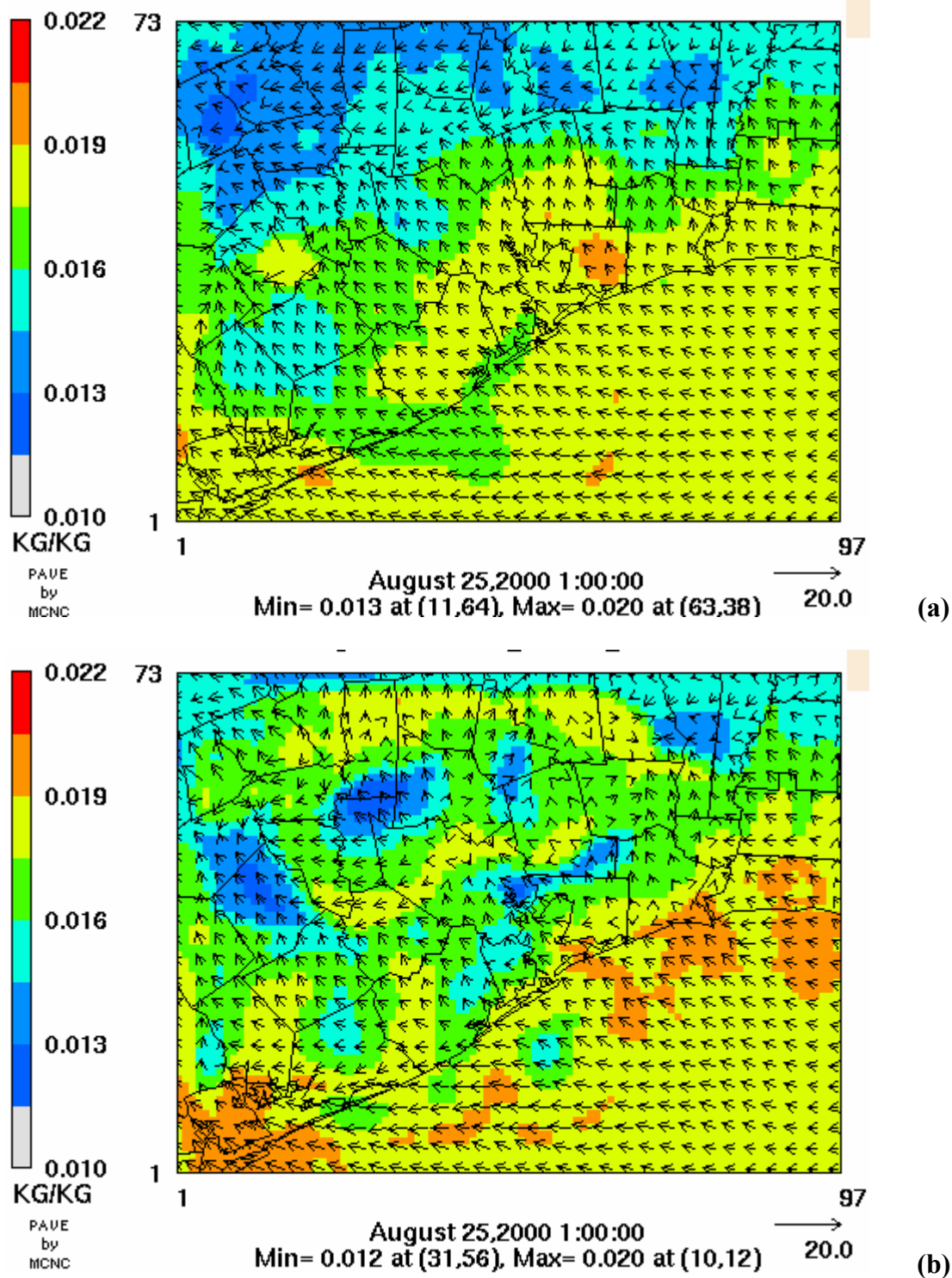


Figure 18. Horizontal distribution of water vapor mixing ratio (kg/kg) and its vector fluxes (m/s kg/kg) at 0100 UTC 25 August 2000 for the (a) “Base” and (b) “Sat” cases.

2.4 Simulate Mesoscale Circulations Using the MM5 (Task 4)

After entirely completing Tasks 2 and 3, we will reconfigure the MM5 with the best physical options and data assimilation methods to generate the most accurate simulations of meteorological fields. We plan to finish Tasks 2, 3, and 4 by the end of the first project year. At that time, we will prepare complete descriptions of our findings on the MM5 simulations and of the process we used to generate meteorological fields for input to the MAQSIP-VGR for simulating ozone and aerosol concentrations during an air pollution episode that occurred from August 23 through September 2, 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) enhancing the SMOKE configurations to handle the variable grids in the MAQSIP-VGR, and (2) acquiring offshore-point-sources data and using them to update our emission inventory for the proposed MAQSIP-VGR simulations. The status of these two subtasks is given below.

2.5.1 Enhancing the SMOKE Configuration

There are 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 for the variable-grid definitions to 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 the 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 will start working on these aspects in the upcoming months.

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 in January 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 the 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 MMS will also be included in updating our emissions database. After completing this task, we will use SMOKE to prepare emissions estimates for use in the MAQSIP-VGR.

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

During this reporting period, we began extending the representation of cloud effects in the MAQSIP-VGR by developing and adapting modules to represent the effects of deep convection and resolved-scale clouds on simulated pollutant distributions. Modules for these cloud processes used in the regular-grid version of the MAQSIP were adapted for inclusion in the MAQSIP-VGR. The convective cloud parameterization is based on the diagnostic cloud module used previously in the Regional Acid Deposition Model (Dennis et al., 1993; Chang et al., 1987; Walcek and Taylor, 1986); these clouds can be either precipitating or nonprecipitating. The module determines whether precipitating or nonprecipitating clouds exist over a grid cell based on input precipitation data derived from the MM5 convective cloud module. Based on the recent Community Multiscale Air Quality (CMAQ) (Byun and Ching, 1999) model implementation of this scheme, only convective precipitation amounts from the MM5 are used to drive the precipitating cloud module; nonconvective amounts are used in the resolved cloud module (Roselle and Binkowski, 1999). Details on the convective cloud parameterization can be found in the references cited above.

The resolvable-scale cloud scheme will be used at all grid resolutions in order to model the scavenging (and aqueous-phase chemistry, in future versions) of pollutant species in the nonconvective layer and resolved clouds. The current implementation assumes the presence of resolvable-scale clouds when condensed water exceeds 0.05 g/kg in a given model grid cell, which represents about one-tenth of the amount needed for autoconversion to precipitation. Scavenging is carried out for all condensate concentrations exceeding this value, and wet removal is computed for times when precipitation fell. Wet removal is modulated by rainout below cloud using an approach similar to that for deep convection. Since our initial MAQSIP-VGR applications in the first year of the project will focus on O₃ and photochemical species simulations, the initial adaptation of the cloud module does not currently include aqueous reactions. However, these will be included in subsequent versions.

Initial testing of this cloud scheme implementation for the MAQSIP-VGR involved a series of 1-D column model tests in which an initially specified vertical pollutant mixing ratio distribution was subjected to cloud processes (mixing, scavenging, and deposition). In these tests we created input data files for the 1-D model by extracting (from prior 3-D data sets) vertical profiles of relevant meteorological data for a single grid cell at which precipitation occurred. The 1-D column model was run such that all physical and chemical processes except clouds were switched off. A variety of tests were conducted that constituted consistency checking of the code. Pollutant vertical profiles were examined before and after they were subjected to these cloud processes to determine the correctness of the implementation. The tests included (1) verification that an initially specified “well-mixed” pollutant field was retained after it was subjected to cloud mixing in the absence of any scavenging and wet deposition; (2) verification that the column

total mass of a pollutant did not change with time after it was subjected to cloud mixing; and (3) verification that vertical profiles of water-soluble pollutants were modified only in “cloudy” layers, when cloud mixing was shut off.

Figure 19 shows example analyses of the consistency checking simulations. Figure 19a presents variations in vertical distributions of O_3 for a case in which only cloud mixing is considered. The changes in vertical profiles are consistent with the existence of cloudy layers during the simulation. We also found that for a species with an initially specified uniform mixing ratio, the “well-mixed” pollutant profile was conserved through the 24 hours of the simulation (not shown). Figure 19b presents the variation in total column O_3 mass relative to the initial pass through the 24 hours of the simulation. The changes in total column mass through the 24 hour simulations are negligible. In future months, we will further test the functionality of this cloud module when performing MAQSIP-VGR simulations.

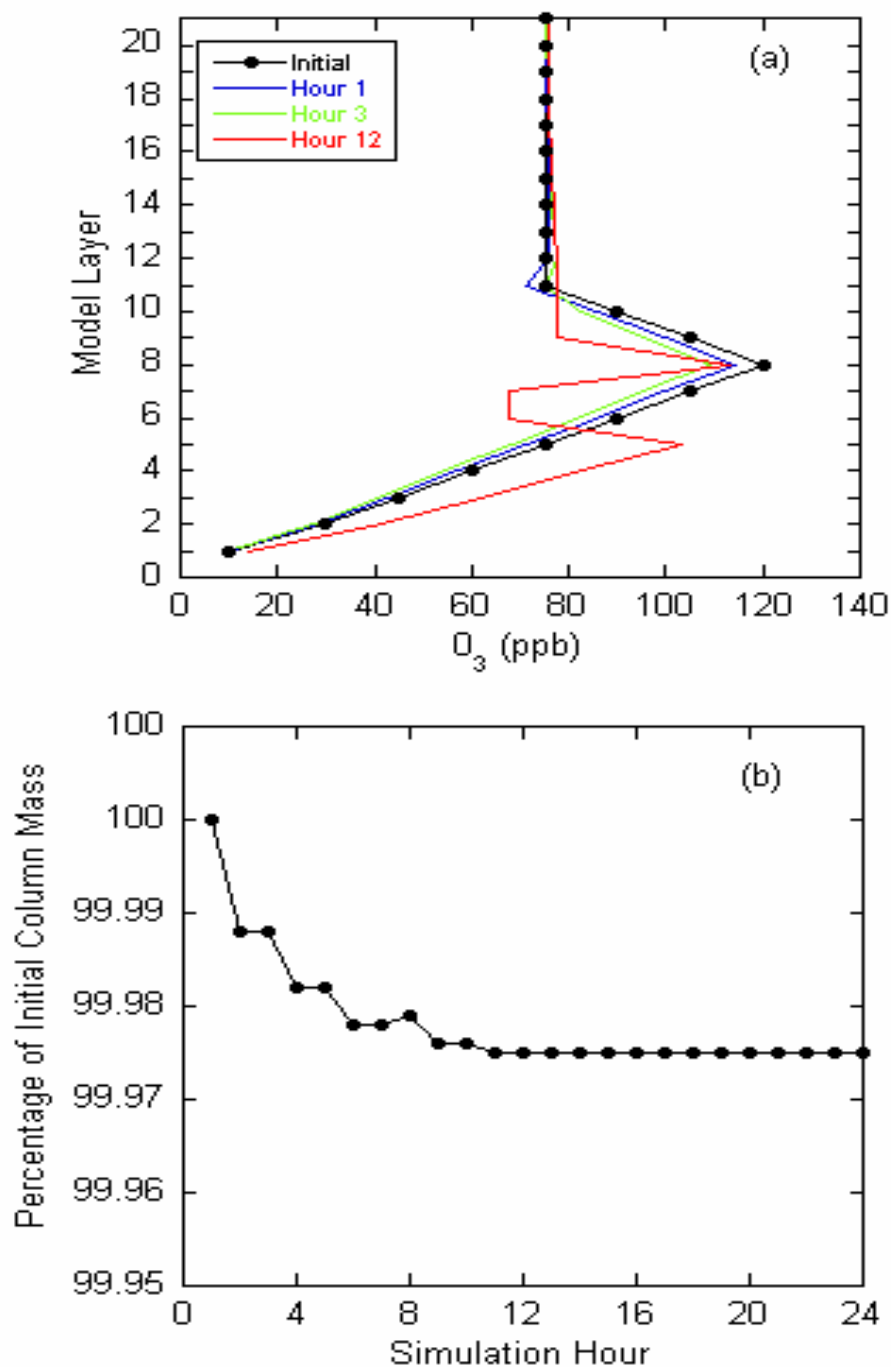


Figure 19. Example results from testing the 1-D cloud module for a case in which an initially specified concentration profile was subjected to cloud mixing. (a) Variation in O_3 vertical profiles at different times during the simulation; (b) change in column total O_3 mass relative to the initial mass.

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

After completing the development of meteorological and emissions inputs suitable for use in the MAQSIP-VGR, we will perform few 10-day simulations (August 23 through September 2) using the MAQSIP-VGR that focuses 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 a same domain but with a very high resolution grid ranging from 400 m to 4 km. These simulations will be completed before the second year of the project.

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, we will perform similar simulations with a focus on the southern Louisiana region (i.e., Domain D04 in Figure 1). Details of this work will be presented in upcoming reports. We plan to complete this task before the end of the second year of the project.

Section 3: Conclusion

Several portions of various tasks were completed successfully during the first six months of this project as per the plan and schedule. Preliminary results from the intercomparison of two different atmospheric boundary layer (ABL) schemes (one using simple, “MRF”, and other using enhanced physics, “Eta”) indicated that usage of better ABL physics resulted in improved meteorological simulations. In the high resolution simulations that will be performed in the future months, we are anticipating better simulations of land-sea breezes and other mesoscale circulations using the “Eta” scheme compared to “MRF” scheme.

Application of our surface data assimilation technique (FASDAS) has resulted in dramatic improvements in the meteorological model simulations. This result will help us improving our understanding of air quality model’s sensitivity to biogenic emission estimations and differing concentrations of hydrogen peroxide on chemical reactions and resulting pollutant concentrations.

Usage of high resolution satellite-derived sea surface temperatures (SSTs) in the meteorological model simulations has resulted in dramatic improvements in precipitation simulations compared to that obtained using a coarse resolution analysis SSTs.

We expect that usage of improved meteorological inputs will lead to improved air quality model simulations. These results will aid us improving our understanding of relative contributions of

onshore and offshore emissions in dictating air pollution over the coastal regions of Gulf of Mexico.

In general, our initial analysis results are highly encouraging, and we look forward to disseminating these results to the atmospheric modeling community after completing more of the project research.

Section 4: Publications

The following conference/workshop presentations resulted from our research during this six-month period:

1. Preliminary Results on the Development of a Variable-Grid-Resolution Air Quality Model. Presented at the *Models-3 Users' Workshop*, October 27-29, 2003, Research Triangle Park, NC.
2. Development of Alternative Methods for Estimating Dry Deposition Velocity in CMAQ. Presented at the *Models-3 Users' Workshop*, October 27-29, 2003, Research Triangle Park, NC.

The work we are completing on several of the project tasks may result in publication of the following journal articles during the first two years of this project (the titles shown are tentative):

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. Effects of Using Satellite-derived Sea Surface Temperatures on Mesoscale Circulations over a Coastal Region and Their Impacts on Air quality Simulations

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