

## APPENDIX B

# DEVELOPMENT OF THE METEOROLOGICAL MODEL

## Appendix B

Table of Contents	Page
Background.....	B-1
Meteorological Run 5d.....	B-3
Diurnal Temperatures.....	B-4
Wind Speeds.....	B-4
Soil Moisture.....	B-4
Vertical Layers.....	B-4
Weather Patterns.....	B-5
Evaluation of the Best Performing Simulation.....	B-5
Meteorological Run 6f.....	B-6
Diurnal Temperatures.....	B-8
Wind Speed.....	B-8
Weather Patterns.....	B-9
Evaluation of the Best Performing Simulation.....	B-9
Final MM5 Configuration.....	B-11
Meteorological Run 5g.....	B-15
Statistical Evaluation of MM5 Run 5g.....	B-20
Processing of MM5 Meteorological Fields for CAMx.....	B-21

## Appendix B

List of Tables	Page
Table B-1 Summary of Meteorological Sensitivity Tests (eight runs).....	B-3
Table B-2 Summary of Revised MM5 Applications.....	B-8
Table B-3 Comparison of Mean Daily Statistics Against Statistical Benchmark for the 4-km Grid.....	B-21
Table B-4 Meteorological Data Requirements for CAMx.....	B-22
Table B-5 Vertical Layer Structure for MM5 and CAMx for Sept. 13-20, 1999 Episode.....	B-23

## Appendix B

List of Figures	Page
Figure B-1	Comparison of Ozone Levels Measured during Baylor University Airborne Sampling Project on September 17 <sup>th</sup> And 18 <sup>th</sup> with Ozone Levels Predicted by Original 1999 Model Simulation Met 3b for Time of Day and Altitude of Flights. (Dotted lines represent collected Ozone data in parts per billion).....B-2
Figure B-2	Observed (black) and Predicted (red) Values for Run 5d For San Antonio/Austin Region.....B-6
Figure B-3	Comparison of the Mixing Height Between the Original Model (Run 4c), 5d, and 6f.....B-3
Figure B-4	Comparison of Wind Speed and Direction, Temperature, Humidity Statistics for Original Meteorological Model Run (black), 5d (red), and 6f (blue) for San Antonio –Austin.....B-11
Figure B-5	Wind Statistics for Original Meteorological Model Run (black), 5d (red), and 6f (blue) for San Antonio-Austin Region.....B-12
Figure B-6	Temperature Statistics for Meteorological Model Run (black), 5d (red), and 6f (blue) for San Antonio-Austin Region.....B-13
Figure B-7	Humidity Statistics for Original Meteorological Model Run (black), 5d (red), and 6f (blue) for San Antonio-Austin Region.....B-14
Figure B-8	Hourly Wind Speeds for Runs 5d and 5g in the 4-km San Antonio Area Domain.....B-16
Figure B-9	Hourly Temperature for Runs 5d and 5g in the 4-km San Antonio Area Domain.....B-16
Figure B-10	Hourly Wind Direction for Runs 5d and 5g in the 4-km San Antonio Area Domain.....B-17
Figure B-11	Hourly Humidity for Runs 5d and 5g in the 4-km San Antonio Area Domain.....B-17
Figure B-12	Comparison of Ozone Levels Measured During Baylor University Airborne Sampling Project on September 17 <sup>th</sup> With Ozone Levels Predicted by 5d and 5g Model Simulation For Time of Day and Altitude of Flights. (Dotted line Represents collected ozone data in parts per billion (ppb)).....B-19

## BACKGROUND

The meteorological inputs used to create the original 1999 episode were developed by ENVIRON using the Fifth Generation Mesoscale Model, referred to as MM5. In their report on development of the 1999 episode simulation, ENVIRON acknowledged certain placement, and precipitation rather well for the September 1999 episode for the entire 4-km domain (South Texas). However, the model only performed marginally when predicting humidity and pressure. Two persistent problems with the original MM5 model simulation, referred to as Met 3b, included wind speed – over predicting of wind speed at night and under predicting during the daytime – and over predicting of early morning temperatures.

The most significant problem in the San Antonio area was aloft wind direction<sup>1</sup>. On September 17 and 18, 1999, air quality sampling was conducted in the San Antonio – Austin area as part of the Baylor University Airborne Sampling Project conducted by TCEQ. The data collected from the Baylor aircraft flights were compared to predictions from the 1999 model simulation for the same days. While the model performed well in replicating peak ozone aloft in the urban plumes for the 17<sup>th</sup> and 18<sup>th</sup>, the spatial distribution was poor, indicating a problem with wind direction at those altitudes. Figure B-1 provides a comparison between the aircraft data and ozone levels predicted by the model for the correct time period and altitude of the flights. On September 17<sup>th</sup> the aircraft took measurements between 600 – 800 meters beginning at 1400 CDT. The flight on September 18<sup>th</sup> began at 1700 CDT and data were collected at about 700 meters during most of the flight. (Emery, et. al., 2002) As shown in the figure, the peak ozone plumes predicted by the model are south of observed plumes for both days that data were collected.

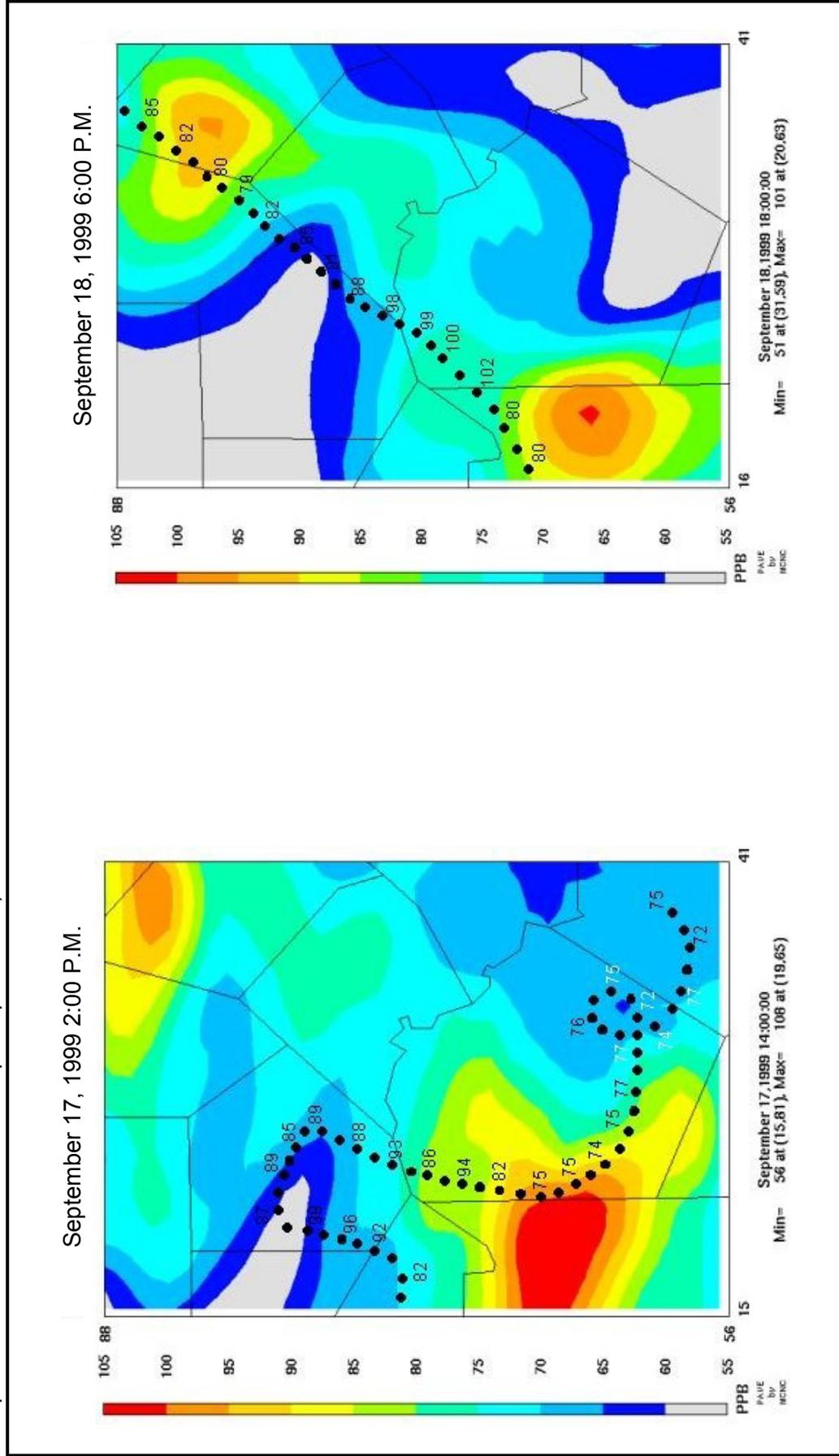
In addition to wind direction issues, simulated ozone levels between the plumes were under predicted by 10 – 20 ppb when compared to observed data. This problem suggests that the model was generating insufficient regional background ozone levels. According to ENVIRON, insufficient background ozone indicates problems with the regional emissions inputs to the model, such as too few VOC emissions from biogenic sources. (Emery, et. al., 2002)

As part of the effort to improve the accuracy of the model, the South Texas Near Non Attainment areas contracted with the ENVIRON and with the University of Texas' Center for Energy and Environmental Resources (UT-CEER) to improve accuracy of meteorological input data for the 1999 episode model.

---

<sup>1</sup> Typically, surface winds transport pollutants locally, while upper (aloft) winds have the potential to transport ozone and its precursors much greater distances, often hundreds of kilometers (APTI).

Figure B-1. Comparison of Ozone Levels Measured during Baylor University Airborne Sampling Project on September 17<sup>th</sup> and 18<sup>th</sup> with Ozone Levels Predicted by Original 1999 Model Simulation Met 3b for Time of Day and Altitude of Flights. (Dotted lines represent collected ozone data in parts per billion.)



ENVIRON, in conjunction with UT-CEER, tested alternative MM5 configurations and parameter algorithms to find the combination that best replicate actual meteorological conditions during the 1999 high-ozone episode. The best of these runs were presented to the air quality planners at TCEQ, and the four NNA partners for further analysis. The runs, labeled 5d, 5g, and 6f, each have unique strengths and weaknesses and impact the photochemical model in various ways, as described below.

**METEOROLOGICAL RUN 5d**

The ENVIRON/UT team conducted eight meteorological runs, labeled 5a, b, c, d, e, f, h, and I, using version 3.4 of the MM5 model while incorporating new databases and model configurations that proved to be successful in other applications throughout the country.

- Change to an alternative boundary layer scheme (Blackadar or MRF) to investigate sensitivity to boundary layer mixing;
- Change to an alternative radiation scheme (RRTM) that is known to perform better in the humid Texas climate and may reduce the morning over-predicted surface temperatures;
- Utilize interactive multi-layer soil moisture schemes now available with the latest release of MM5 (v3.5) that would provide a more realistic feedback between soil and atmosphere; and
- Test the effects of alternative observational analyses and FDDA techniques that may better characterize conditions in the south central U.S.

Table B-1. Summary of Meteorological Sensitivity Tests (eight runs)

Run ID	Configuration
Run 5c	Identical to Run 4c (the best performing of the original runs reported by Emery and Tai, 2002), except that the Blackadar PBL scheme was replaced by the Gayno-Seaman PBL scheme.
Run 5	Identical to Run 5c except that the Dudhia Cloud radiation scheme was replaced by the RRTM radiation scheme
Run 5b	Identical to Run 5 except that data from the Texas Coastal Ocean Observation Network (TCOON) and NOAA National Buoy Center were added to the original observational FDDA input data set.
Run 5d	Identical to Run 5b, except that the MRF PBL scheme replaced the Blackadar PBL scheme.
Run 5e	Identical to Run 5d, except that the standard 5-layer soil model was augmented by the bucket soil moisture option, and Run 5e used the standard climatological default soil moisture to define the initial soil conditions by land use category (up to this point, soil moisture was reduced 25% from standard values as in the original Run 4c).
Run 5f	Identical to Run 5e, except that the reduced soil moisture was used similarly to Runs 4c and 5-5d.
Run 5i	Identical to Run 5d except that the number of vertical layers was increased from 28 to 41, resulting in about twice the vertical resolution between approximately 250 and 4600 meters above the surface.
Run 5h	Identical to Run 5e (bucket soil moisture with standard default initial soil moisture values) except that the number of vertical layers was increased from 28 to 41.

When conducting the eight runs, which are listed on table B-1, modelers tested two methodologies for determining the depth of the planetary boundary layer (the Blackadar and Medium Range Forecast schemes), two radiation schemes<sup>2</sup> (the Dudhia-Cloud and Rapid Radiation Transfer Model), three versions of the four dimensional data assimilation (FDDA) model<sup>3</sup> (versions 11, 12, and 13), three soil moisture schemes, and two vertical-layer<sup>4</sup> resolutions (28 layers versus 41 layers).

### **Diurnal Temperatures**

The Dudhia Cloud scheme overestimated the amount of radiation absorbed and re-radiated by the atmosphere. This resulted in very warm nighttime minimum temperatures. When the RRTM radiation scheme was used rather than the Dudhia Cloud scheme, the simulated temperature range compared very closely with the observed diurnal temperature ranges. The simulated maximum temperatures were too cool compared to the observed maximum temperatures.

### **Wind Speeds**

Wind speeds were analyzed with the Blackadar PBL scheme and the MRF PBL scheme. The Blackadar PBL produced high daytime and nighttime winds, which suggested that the Blackadar approach produced an overly aggressive vertical transfer of momentum. It was also noted that higher winds near the top of the boundary layer may mix to the surface too rapidly. These occurrences can be related to the under prediction of maximum temperatures. The MRF PBL scheme did result in an improved prediction of both daytime and nighttime wind speeds. Nighttime winds were noted to be high however. With the MRF PBL scheme, the daytime maximum temperatures warmed by 1 to 2 K but remained below the observed temperatures.

### **Soil Moisture**

The use of the bucket soil moisture option in the model, rather than the five-layer soil model, produced a consistent increase in wind speed. Maximum temperatures also improved slightly during the final days of the episode.

### **Vertical Layers**

In the modified run, the model was configured to run with 41 layers rather than 28 in order to investigate the effects of increased vertical resolution. Higher resolution (usually more than 30 layers) in the vertical direction is recommended and widely adopted. The run did not indicate improvement in model performance at the boundary layer or at the surface.

---

<sup>2</sup> Shortwave radiation from the sun and longwave radiation from the earth impact atmospheric processes by producing heat, moisture, and momentum exchanges, which drive the PBL.

<sup>3</sup> Four dimensional data assimilation (FDDA) refers to a sophisticated method of initializing a predictive model such as MM5. MM5 and similar models estimate meteorological processes using numerical equations. To make numerical forecasts, the models must have a starting point in which initial conditions are provided in the form of gridded data. FDDA combines numerical predictions with observations to provide a 4-dimensional estimate of initial meteorological parameters. The FDDA technique utilized to develop the refined 1999 episode was the “nudging” technique in which the model is gently pushed toward observed values using numeric equations.

<sup>4</sup> The modeling team employed the “Sigma Coordinate System” in which the lowest vertical coordinate follows a smoothed version of the actual terrain. The higher sigma surfaces parallel the lowest coordinate but gradually transition to being nearly horizontal at the top of the coordinate system, typically above the tropopause. When 28 sigma levels are used, the 8 lowest layers make up the planetary boundary layer. By increasing the vertical layers to 41, additional vertical layers are focused in the boundary layer and jet stream, which provides a higher resolution than the 28-layer system.

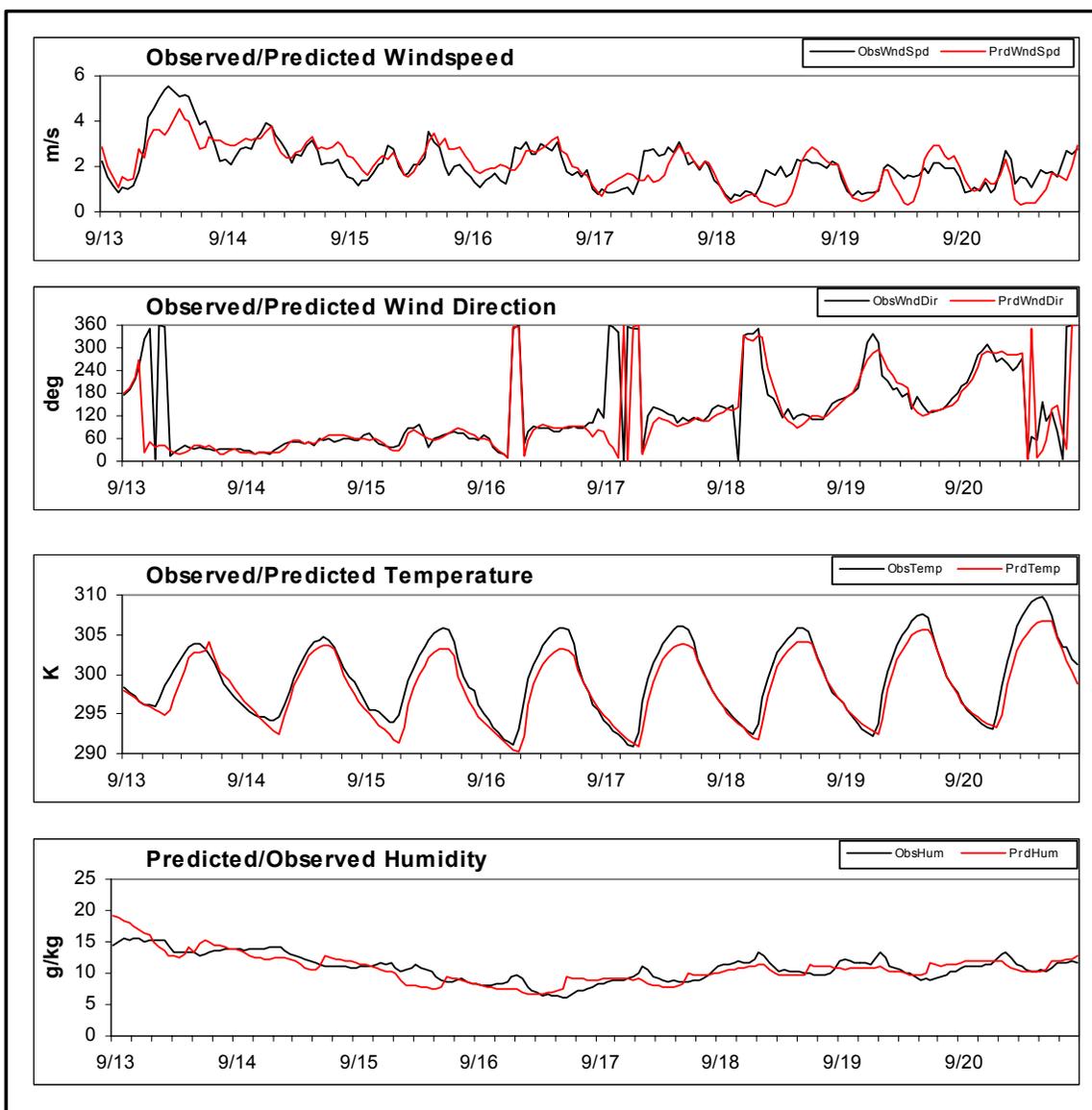
### **Weather Patterns**

Surface pressure patterns predicted by both the Blackadar and MRF runs compared well with observed pressure patterns. Cloud type and coverage across the domain were similar, however the Blackadar runs produced greater amounts of low-level cloudiness over South Texas and Gulf of Mexico on some of the modeling days. Rainfall amounts was not predicted after the 14<sup>th</sup> of September, which was in concurrence with the observed rainfall levels. A deeper mixed layer was produced by the MRF PBL scheme than the Blackadar runs with heights greater by 25% - 35%.

### **Evaluation of the Best Performing Simulation**

Overall, run 5d produced the best results of the eight sensitivity runs. Wind speed and wind direction improved when comparing run 5d results with the meteorological inputs used in the original 1999 simulation. However, 5d maintained a northerly wind bias throughout much of the episode. Run 5d predicted cooler daily temperatures than observed; but daily minimum temperatures were much closer to observed values than those predicted by other runs. Humidity resulted as erroneous predictions and may be a cause for concern not on model performance but rather errors in the simulation of spatial and temporal evolution of the boundary layer by the PBL scheme, particularly along the coast line. Figure B-2 provides a comparison between observed and predicted (run 5d) wind speeds, wind direction, temperature, and humidity in the San Antonio – Austin region during the September 1999 episode. As shown, there was a high degree of correlation between observed and predicted values for these four meteorological variables.

Figure B-2. Observed (black) and Predicted (red) Values for Run 5d for San Antonio/Austin Region



### METEOROLOGICAL RUN 6f

The ENVIRON/UT-CEER team also developed a series of meteorological runs which took advantage of new / additional input data from EPA as well as the expanded capabilities of MM5 version 3.5. Improvements within version 3.5 included improvements within known deficiencies and to access additional modeling capabilities. These modifications included:

1. The same four-domain nested mesh with 108/36/12/4-km resolution, but with an expanded 36 km grid in order to move possible 108/36 boundary artifacts away from the area of interest and to better simulate the dominant regional-scale

meteorology over the entire central U.S. that dictated flow and pressure patterns in Texas during the episode.

2. The coupled Pleim-Xiu Land Surface Model and boundary layer model, which required additional datasets such as soil type, vegetation categories, deep soil temperature, and vegetation fraction archived at the National Center for Atmospheric Research.
3. Three-hourly observational “analysis” fields from the Eta Data Assimilation System, (EDAS) as opposed to EDAS “initialization” data used in previous modeling to establish initial/boundary conditions and inputs to the MM5 Four Dimensional Data Assimilation (FDDA) package.
4. Incorporation of routine surface and upper-air observation data obtained from NCAR archives into the EDAS fields processed for each MM5 modeling grid. This modification was made to ensure that the mesoscale and local meteorological features in the south-central U.S. were faithfully characterized in the EDAS analysis dataset. This preprocessing step was skipped in the original application because it was believed that the relatively high spatial and temporal resolution of the EDAS fields was sufficient to capture these details.
5. Use of the RRTM radiation scheme for all grids, based on the favorable results from the sensitivity tests.
6. Use of two-way interactive nesting for all grids. The 4-km grid was run as an independent one-way nest in the original application.
7. Modifications to the FDDA nudging technique to include two-dimensional surface analysis nudging, altered nudging strengths, and recommendations of Dr. Nelson Seaman at the Pennsylvania State University. The TCOON and NOAA buoy data were also added to the observation FDDA nudging inputs.

These capabilities were not available in version 3.4 of MM5 used to develop the original 1999 simulation, nor were they addressed in runs 5a – 5i. The new runs, labeled 6c – 6f, were each modified to reflect different parameters applied to each run.

Runs 5a – 5i contained a 36 –km grid system that was arranged in 55 X 55 grid cells. The “run 6” series used an expanded 36-km grid system that covered 85 X 61 grid cells. All nested grids within the 108-, 36-, 12-, and 4-km grid system, were run in two-way interactive mode.<sup>5</sup> In contrast, the run 5 series incorporated one-way interaction<sup>6</sup> on the 4-km grid, with 2-way interaction on other nested grids. All “6 series” runs were conducted with 28 vertical layers, since the run 5 series results indicated this resolution performed best.

---

<sup>5</sup> Finer resolution grids are nested inside of coarser-resolution grids. The information for the outermost grid is supplied from an outside source using one-way interaction. The coarse grids provide boundary conditions on the mesh interfaces between coarse/fine grids. Forecast variables developed in the fine grids are used to update the coarse grids that they cover, resulting in two-way interaction since information flows from coarse to fine grid as well as from fine grid to coarse grid.

<sup>6</sup> In one-way interaction, information flows in one direction: from the coarser grid system to the finer grid system. Computations within the fine model do not affect the larger grid system.

Cloud options remained consistent with runs 4 and 5, which mainly consisted of treating cloud microphysics with the “simple ice” mechanism.

The run 6 series also varied by the grids in which the settings were modified. For example, the sole difference between runs 6c and 6e was that 6e included initial / boundary condition modifications applied to all grids, whereas these modifications were only applied to the three largest grids in 6c.

ENVIRON/UT also employed a Land Surface Model to improve handling of surface-atmospheric interactions for the run 6 series. The more sophisticated Land Surface Models (LSMs) would provide advantages for mesoscale modeling than did the simple “five-layer” soil model. Surface-atmosphere processes affect the magnitude and direction of sensible and latent heat transfer which then defines boundary layer development, surface temperature, and humidity which are important for successful air pollution modeling. The Pleim-Xiu approach was reputable for outstanding results in air quality planning in other parts of the county therefore was utilized in correlation with the MM5 application.

In addition, the modeling team incorporated supplemental data sets, such as soil type, vegetation categories, and deep soil temperature. The following information describes the revised MM5 applications.

Table B-2. Summary of Revised MM5 Applications

Run ID	Configuration
Run 6c	Includes 2-D surface nudging toward wind, temperature, and humidity analyses, and soil moisture nudging toward surface humidity
Run 6d	Identical to Run 6c, except soil moisture nudging was turned off
Run 6e	Identical to Run 6c, except 2-D analysis and soil moisture nudging was applied to the 4 km domain
Run 6f	Identical to Run 6e, except with additional surface observations from TCOON and NBDC buoy sites in the observation nudging database.

### Diurnal Temperatures

The diurnal temperature range was suppressed, resulting in cooler afternoon maxima and warmer morning minima. In run 6d, temperatures improved significantly when the soil moisture nudging was turned off yet still produced worse results than in run 4c. Run 6e had comparable diurnal temperatures to the 4c original run.

### Wind Speed

Wind speed trends in run 6c were much better simulated than in the 4c original run. The speeds were stronger in the afternoon and lighter at night. The first four days of the simulation had wind speeds that were overpredicted. However, wind speeds during September 17<sup>th</sup> through September 20<sup>th</sup> corresponded well to the observed wind speeds. Run 6d resulted in stronger wind speeds. Run 6e predicted wind speeds and direction which were compatible to observed levels.

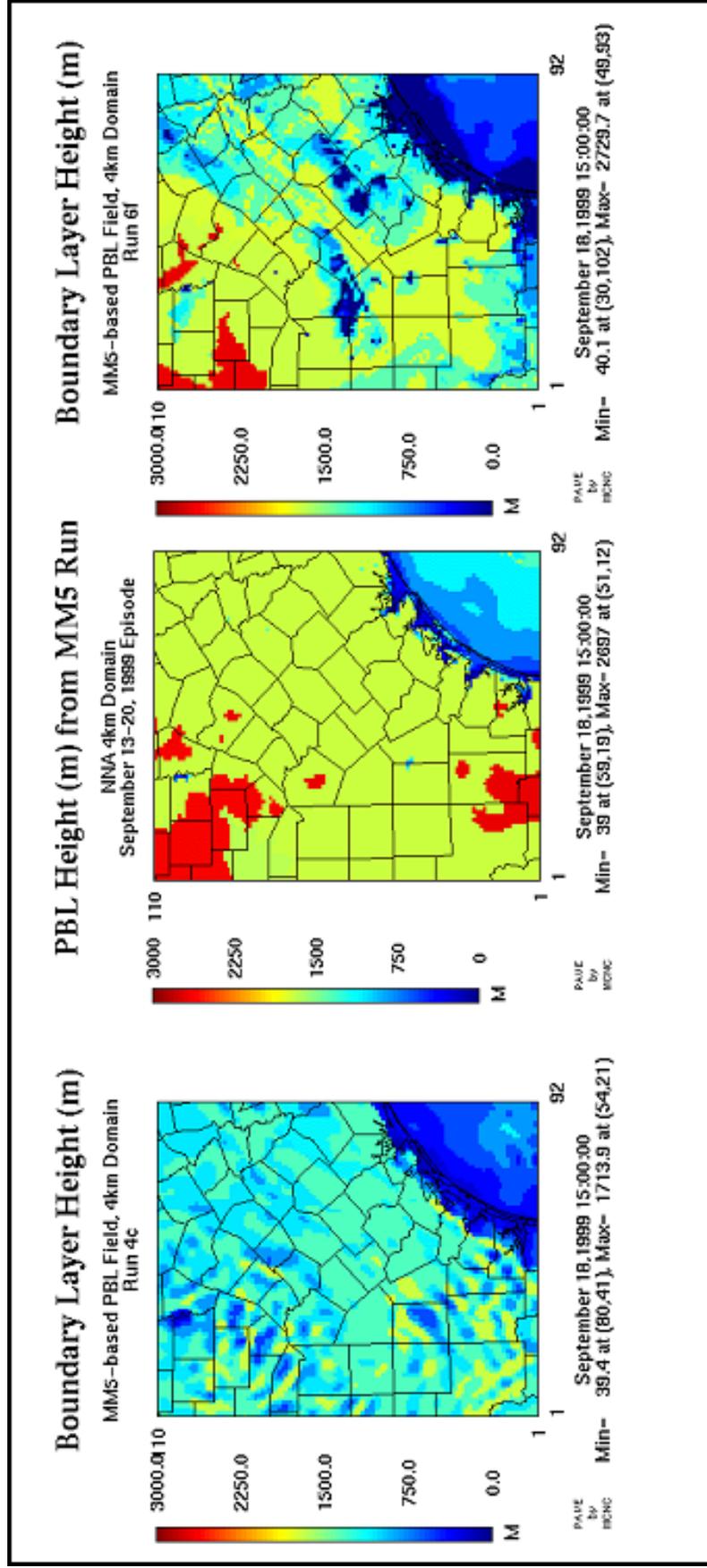
**Weather Patterns**

Diurnal trends of moisture were not predicted well in run 6c as compared to the run 4c. Run 6d had poor moisture performance on all modeling days. Humidity in run 6e was generally higher than the other runs but most closely matched observed values.

**Evaluation of the Best Performing Simulation**

The final run, 6f, incorporated additional surface observation data from the Texas Coastal Ocean Observation Network and the National Buoy Data Center. Of this series, run 6f was considered the best performing simulation. Run 6f predicted temperature and humidity more accurately than 5d and demonstrated improved wind speed and wind direction when compared to the original 1999 simulation. However, the improved wind statistics for 6f were inferior to the improvements demonstrated by 5d. Furthermore, the boundary layer patterns from 6f were considered questionable. (ENVIRON, 2003) This is shown graphically in figure B-3, which compares the mixing height between the original model, 5d, and 6f. The graph for 6f displays an area of suppressed mixing that appears to track a swath of sandy soil from southern San Antonio to Bryan, Texas. According to ENVIRON, this indicates the run 6f configuration was excessively sensitive to sandy soil.

Figure B-3. Comparison of the Mixing Height Between the Original Model (Run 4c), 5d, and 6f



### FINAL MM5 CONFIGURATION

Overall, the ENVIRON/UT-CEER team considered run 5d to outperform all other 5 and 6 series runs. Their conclusions were based on measurements as to how accurately the runs simulated observed conditions as well as other performance statistics. These performance results are shown in figures B-4 through B-7. Figure B-4 provides a comparison of observed wind speed, wind direction, temperature, and humidity with values predicted by the original meteorological model, run 5d, and 6f. Figures B-5 through B-7 provide statistical measures of performance for wind speed / direction, temperature and humidity, respectively.

Figure B-4. Comparison of Wind Speed and Direction, Temperature, Humidity Statistics for Original Meteorological Model Run (black), 5d (red), and 6f (blue) for San Antonio – Austin

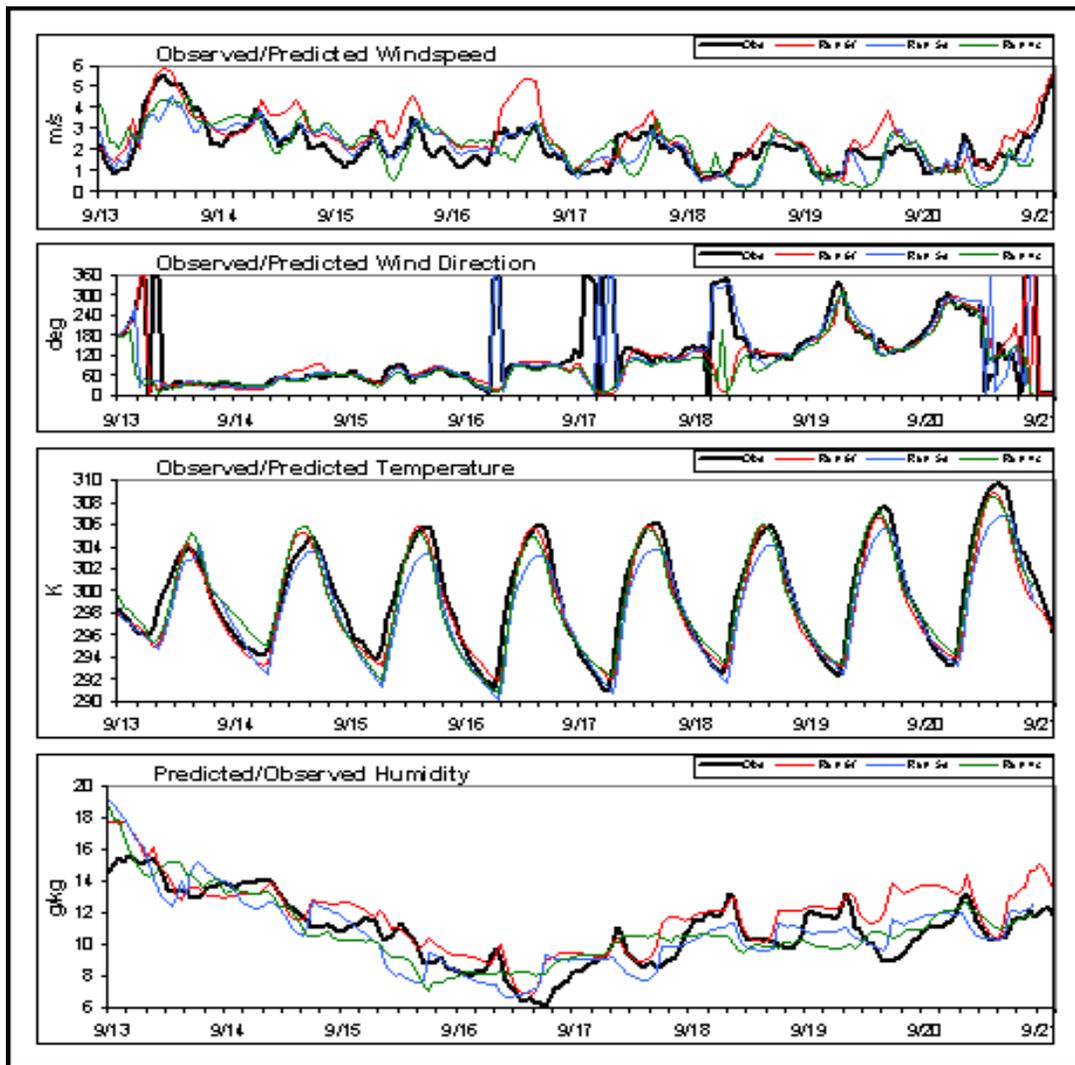


Figure B-5. Wind Statistics for Original Meteorological Model Run (black), 5d (red), and 6f (blue) for San Antonio – Austin Region

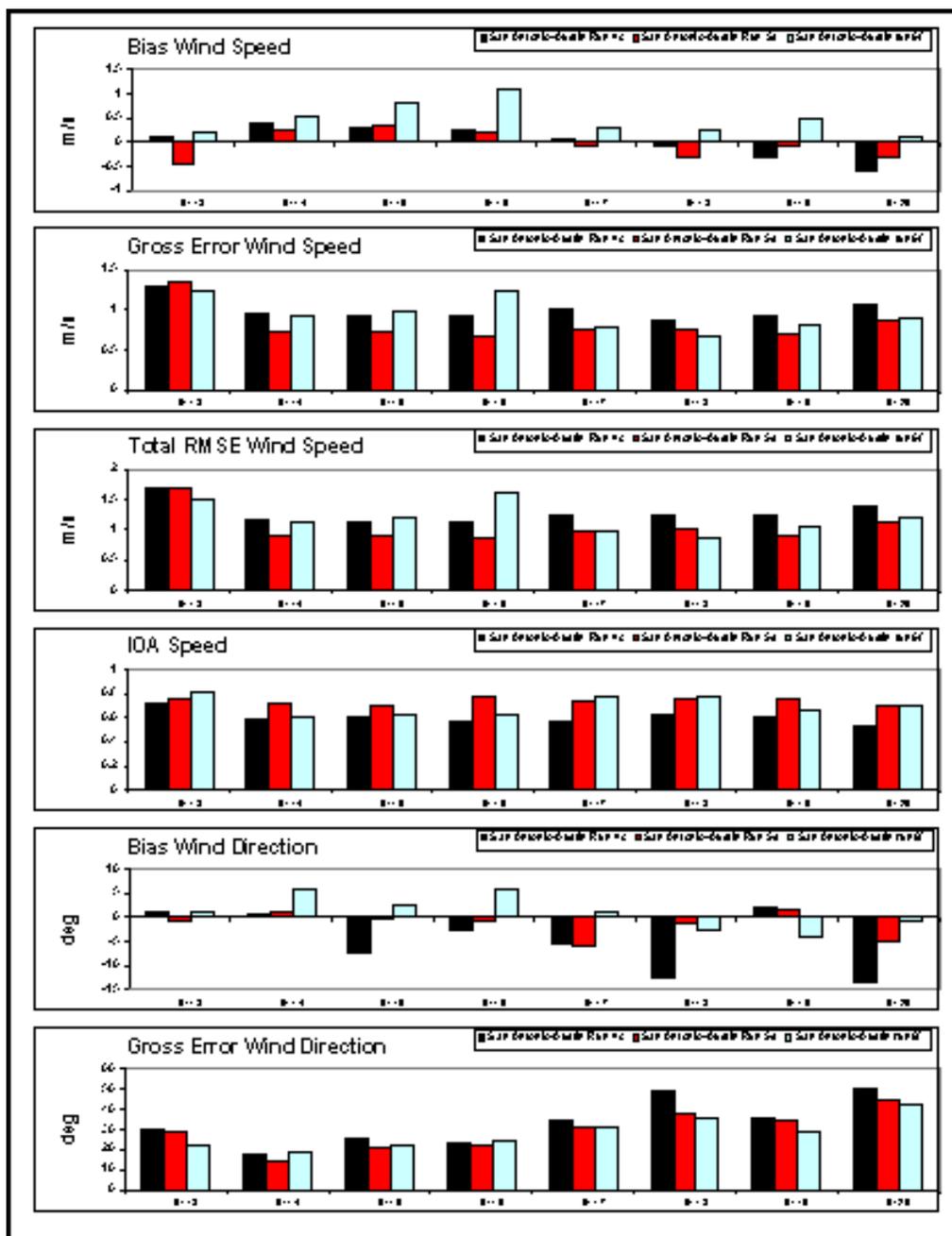


Figure B-6. Temperature Statistics for Meteorological Model Run (black), 5d (red), and 6f (blue) for San Antonio – Austin Region

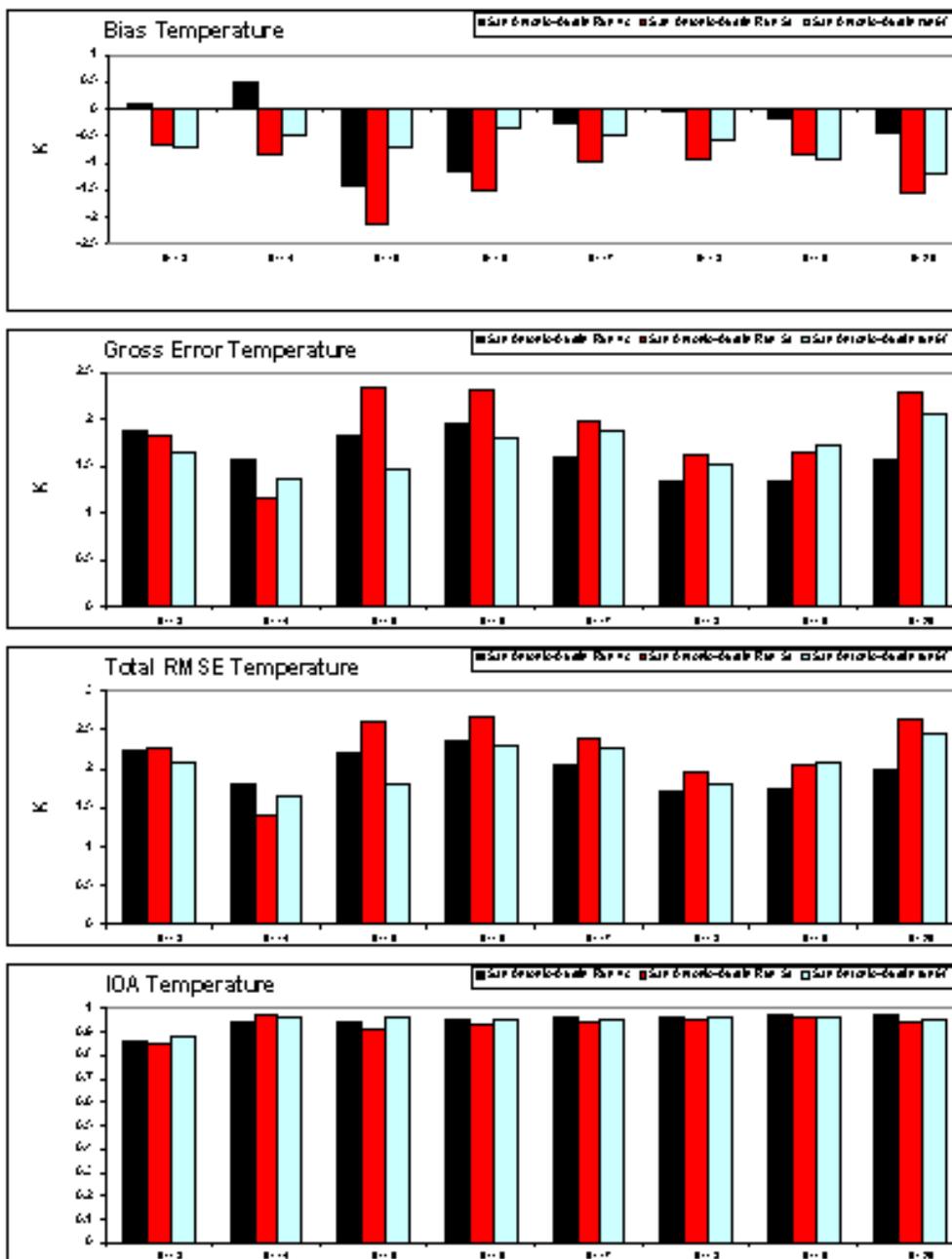
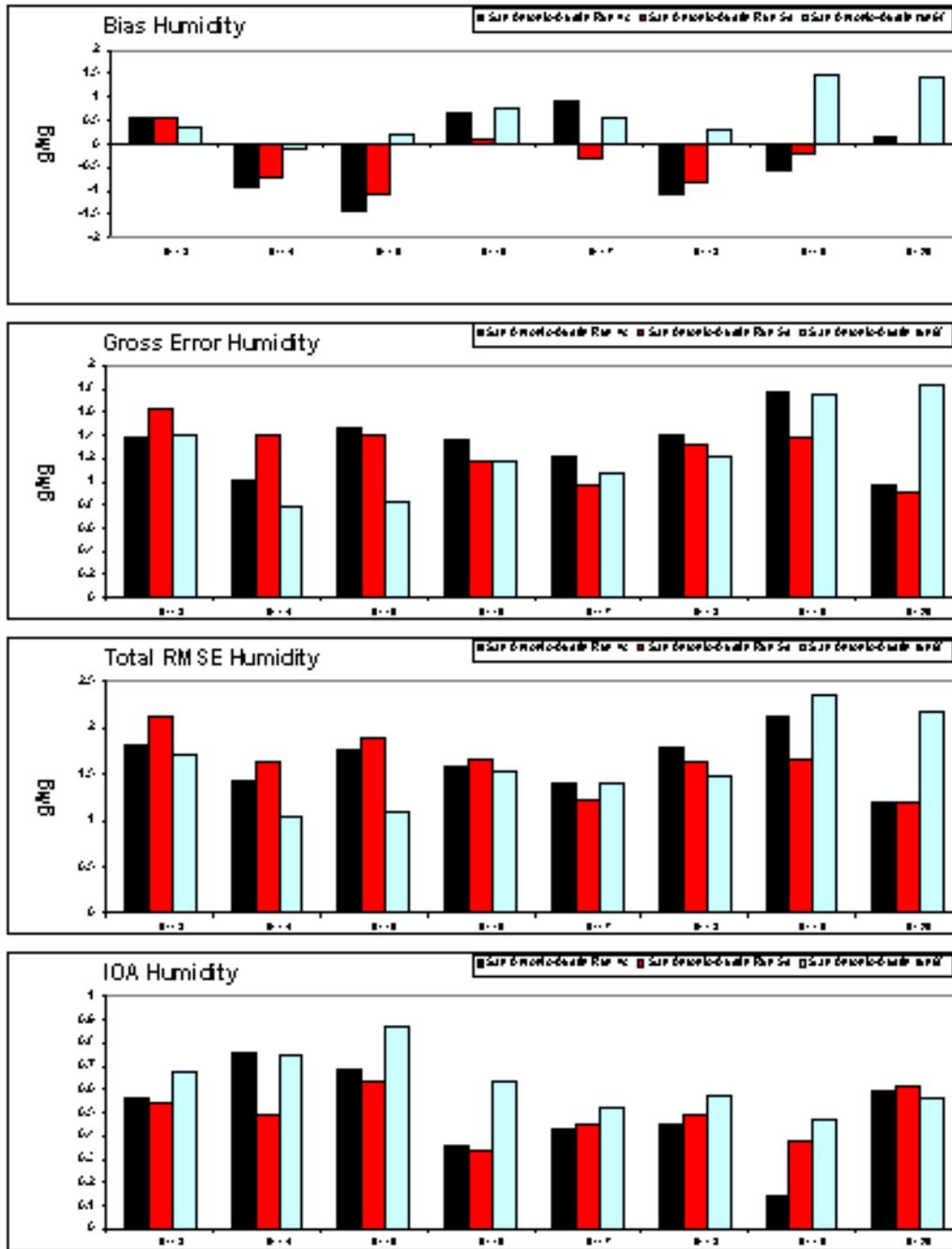


Figure B-7. Humidity Statistics for Original Meteorological Model Run (black), 5d (red), and 6f (blue) for San Antonio – Austin Region



### **METEOROLOGICAL RUN 5g**

The ENVIRON/UT-CEER team undertook one additional run to merge the best configurations of the 5 and 6 series runs. The team recommended that the MM5 Run 5d set of meteorological fields for the photochemical model be used in combination with important FDDA and input database changes adopted in MM5 Run 6f, but the MRF PBL scheme and five-layer soil model of Run 5d be maintained. This configuration included:

- 28 sigma levels
- Expanded 36-km domain used in Run 6f
- Two-way interactive 108/36/12/4-km grids
- FDDA analysis nudging on the 108/36/12-km grids:
  - 3-D analysis nudging: MM5 was lightly nudged toward 3-hourly gridded EDAS analysis of winds (in the boundary layer and aloft) and temperature and humidity (only above the boundary layer), which were improved by the blending of routine surface and upper-air observational data
  - 2-D surface analysis nudging: MM5 was lightly nudged toward 3-hourly gridded surface analyses of winds, temperature, and humidity generated by the RAWINS program.
- Observation nudging on the 12/4-km grids: MM5 was strongly nudged toward discrete hourly wind observations from routine and special measurement networks operating in Texas during the episode.
- MRF PBL
- Simple ice cloud microphysics
- Kain-Fritsch cumulus parameterization except on 4-km grid
- Five-layer soil model
- RRTM radiation scheme
- Reduced soil moisture and thermal inertia to account for drier conditions

The results of run 5d and 5g are very comparable; for example, both runs predicted similar PBL heights. However, there were strengths / weaknesses found in both models. Run 5g out-performed 5d in terms of predicting temperature and humidity. Conversely, run 5d out-performed 5g in terms of wind speed and ground-level wind direction. Run 5g wind speed and direction predictions for Central Texas during the first half of the episode were slightly degraded compared to Run 5d; however, along the coast, Run 5g showed enhanced onshore afternoon flow that was in better agreement with observations. Figures B-8 through B-11 provide comparisons of wind speed, wind direction, temperature, and humidity, between observed values and values predicted by runs 5d and 5g.

Figure B-8. Hourly Wind Speed for Runs 5d and 5g in the 4-km San Antonio Area Domain

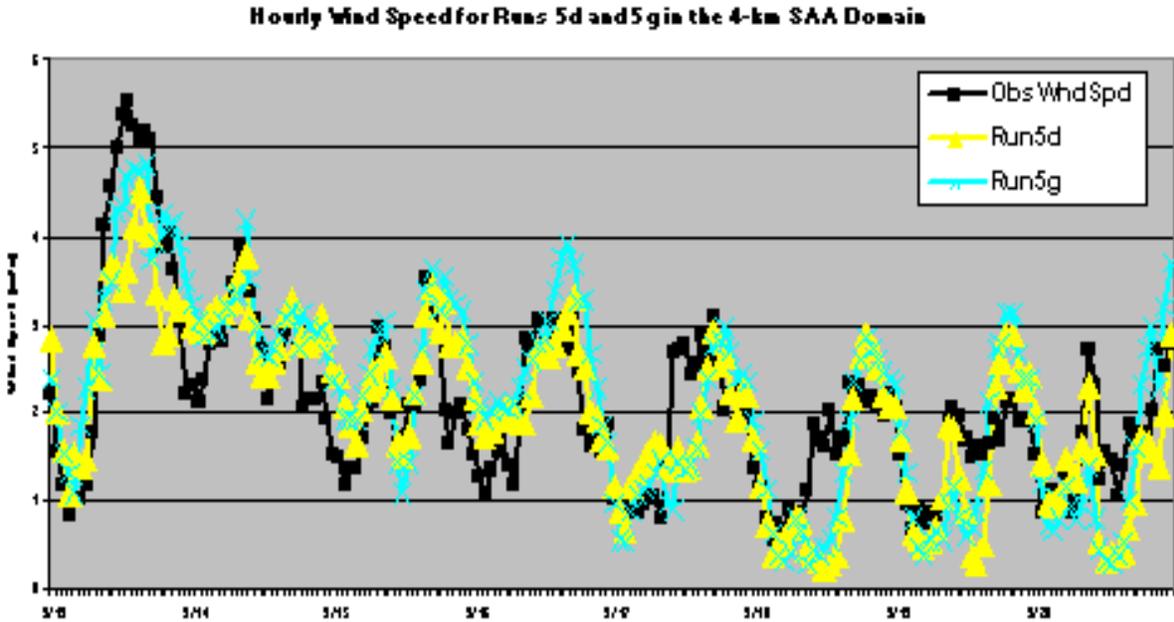


Figure B-9. Hourly Temperature for Runs 5d and 5g in the 4-km San Antonio Area Domain.

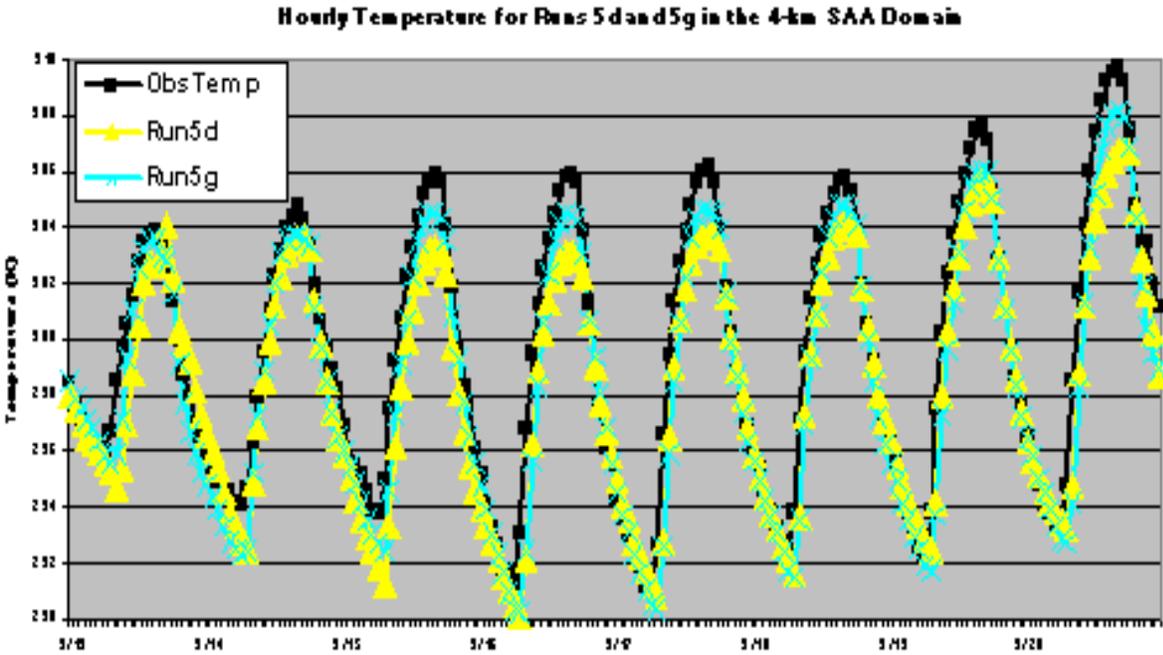


Figure B-10. Hourly Wind Direction for Runs 5d and 5g in the 4-km San Antonio Area Domain

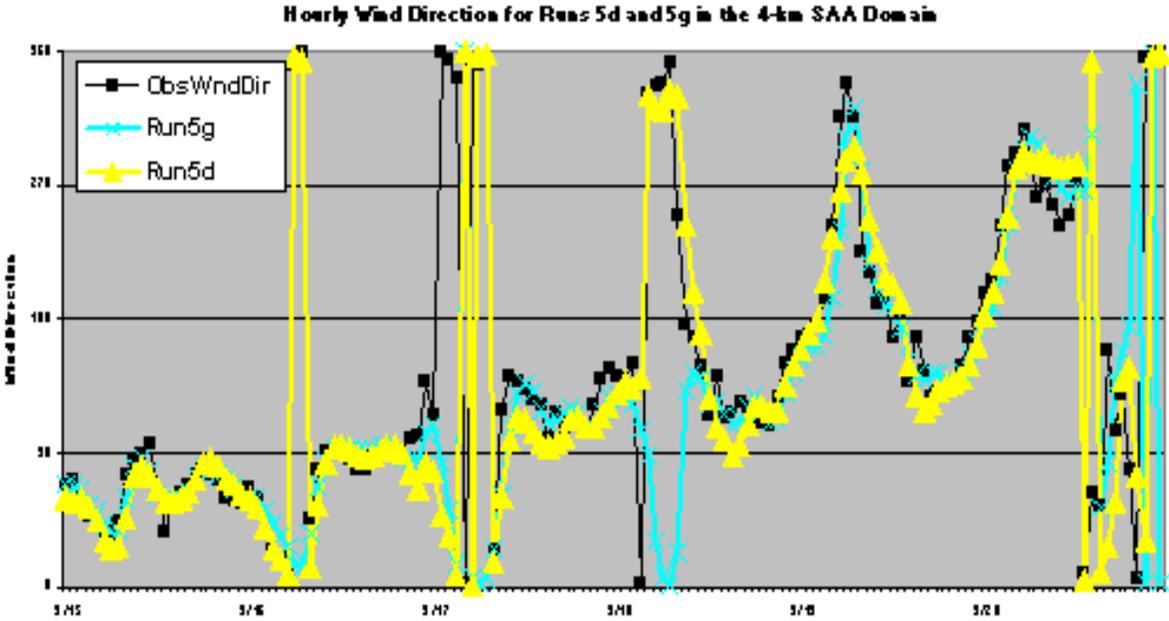
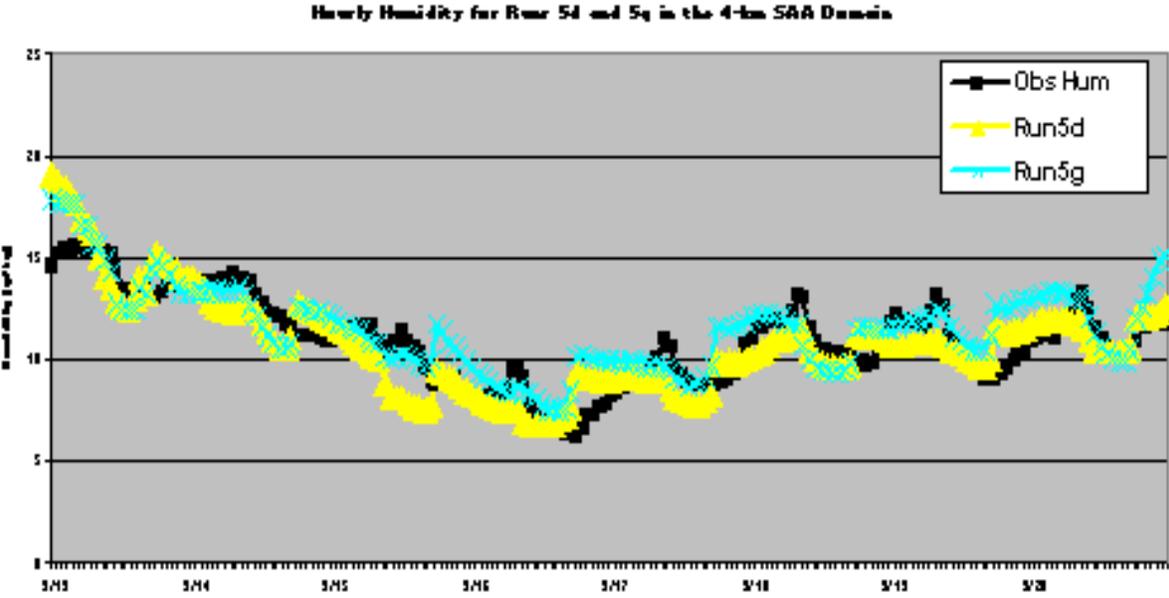


Figure B-11. Hourly Humidity for Runs 5d and 5g in the 4-km San Antonio Area Domain.

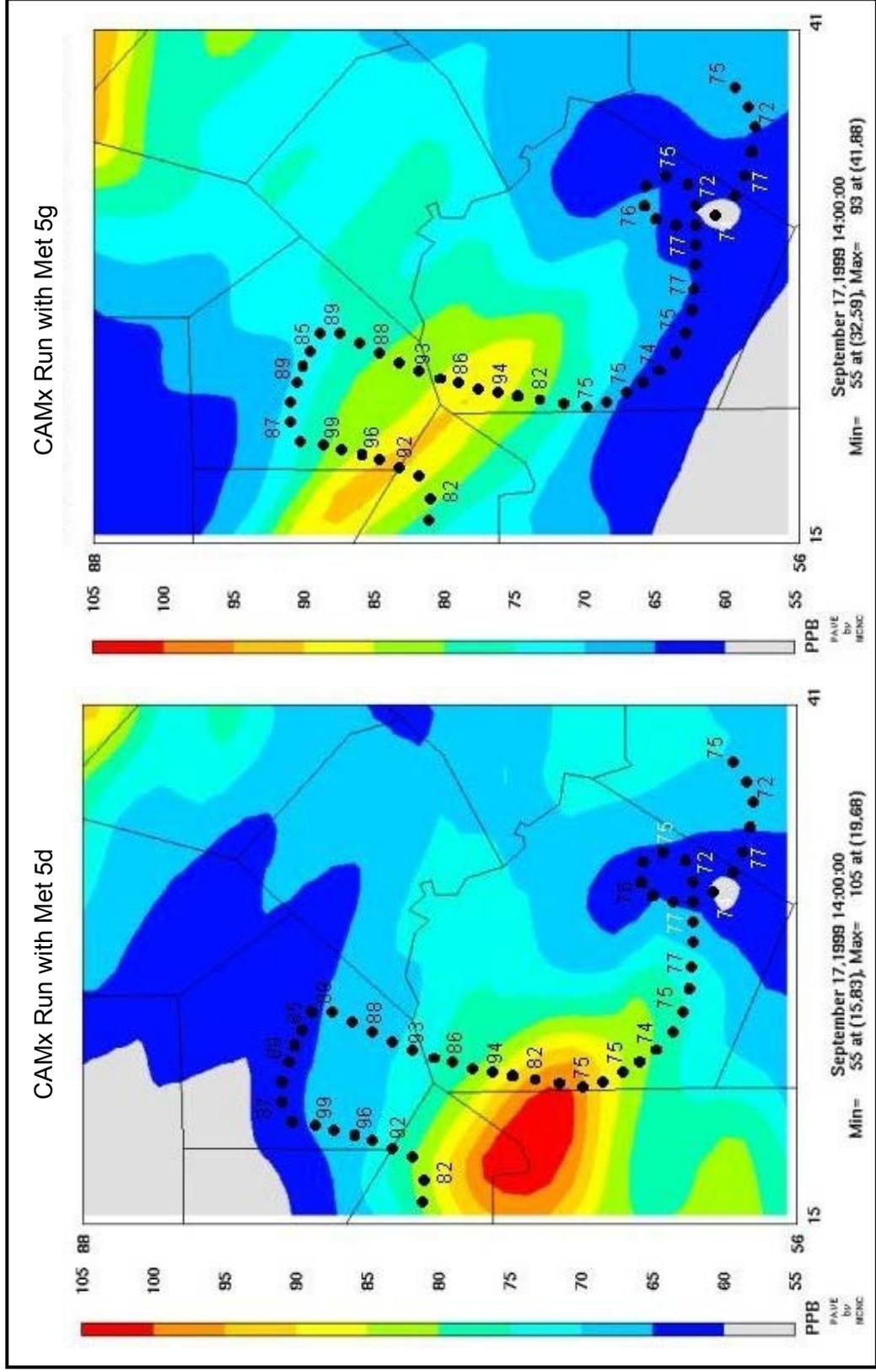


Since the results of the 5d and 5g wind speed/direction, temperature, and humidity comparisons were inconclusive in terms of which one was the superior meteorological

run, additional analyses were conducted. These included running the two meteorological simulations through the CAMx photochemical model to determine the impact each run had on predicting ozone levels; and further, comparing the photochemical results to the Baylor aircraft sampling data for the time and altitude of the flights. The two photochemical runs, labeled run 14 (using the 5d meteorological run) and run 16 (using the 5g meteorological run) were identical with the exception of the meteorological inputs.

A problem that was significant in the San Antonio area was aloft wind direction. While the model performed well in replicating peak ozone aloft in the urban plumes with the original Met 3b run for the 17th and 18th, the spatial distribution was poor, indicating a problem with wind direction at those altitudes. The data collected from the Baylor aircraft flights were compared to predictions from the 1999 model simulation for the same days for Met Run 5d and 5g. Figure B-12 provides a comparison between the aircraft data collected by Baylor University and ozone levels predicted by the model for the correct time period and altitude of the flights. As shown in the figure, the peak ozone plumes predicted by the model are vastly improved.

Figure B-12. Comparison of Ozone Levels Measured during Baylor University Airborne Sampling Project on September 17<sup>th</sup> with Ozone Levels Predicted by Met 5d and 5g Model Simulation for Time of Day and Altitude of Flights. (Dotted line represents collected ozone data in parts per billion (ppb).)



## **STATISTICAL EVALUATION OF MM5 RUN 5g**

The University of Texas at Austin provided the following information regarding the statistical evaluation of the MM5 model performance. Winds, temperature, and humidity were quantitatively assessed to analyze MM5 performance at all available surface observation stations across the 4-km domain. The METSTAT program developed by ENVIRON (2001) was utilized for the evaluation. The METSTAT program generates pairing of observations and predictions and calculates statistical measures for wind speed, wind direction, temperature, and humidity. The following statistical metrics were examined:

- Bias error – mean difference between pairings of predicted and observed data over a region.
- Gross error – mean absolute value of difference between pairings of predicted and observed data over a region.
- Root Mean Square Error (RMSE) – the square root of the mean of the squared difference between pairings of predicted and observed data over a region.
- Index of agreement (IOA) – at each monitoring site, calculate the sum of the absolute value of the difference between the prediction and the mean of the observations and the absolute value of the difference between the observation and the mean of the observations. These sums are added over all monitoring sites and divided into the square of the RMSE. This value is then subtracted from one.

Performance goals for the above parameters were established from a comparison of statistical summaries of the results of nearly thirty regional meteorological model simulations used to drive photochemical models throughout the country. Performance goals were chosen to establish a level of performance that most past modeling has achieved and to filter out those applications that exhibit particularly poor performance. It should be stressed that these goals are guided by the results of meteorological models that have been accepted and used in support of historical regulatory photochemical air quality modeling efforts. The performance goals will require refinement as the state of the science of meteorological modeling improves.

Comparisons of mean daily statistics on the 4-km grid against the statistical benchmarks are summarized in table B-3 for the San Antonio/Austin, Corpus Christi/Victoria, and Houston/Galveston sub-domains. The importance of the various meteorological input fields on CAMx air quality modeling can be ranked as follows (in descending order):

1. Surface and vertical profiles of wind speed/direction;
2. Boundary layer mixing depth and intensity;
3. Temperature (primarily the extent to which it influences boundary layer characterization, but secondarily, the extent to which it affects chemical reaction rates);
4. Humidity and clouds (assuming cloud cover was insignificant, which was the case during this episode).

The table B-3 reveals that excellent performance for wind speed and direction and good performance for temperature and humidity was achieved by the Run 5g simulation on the 4-km domain. The reader is cautioned that these results are based on comparisons to observations obtained from ground-level monitoring stations. Upper air observations

in the 4-km domain were limited to two locations. Vertical profiles of observed wind, temperature, and humidity were available from the Corpus Christi National Weather Service rawinsonde station. Vertical profiles of boundary layer winds were available from a special air quality study (Big Bend Regional Aerosol and Visibility Observational) profiler located in Llano, Texas. Run 5g and Run5d achieved the best performance at these two monitoring stations.<sup>7</sup> (EMERY, C.A., et. al., 2003)

Table B-3. Comparison of Mean Daily Statistics Against Statistical Benchmark for the 4-km grid.<sup>8</sup>

Parameter	Benchmark	Episode Mean		
		Austin/ San Antonio	Corpus Christi/ Victoria	Houston/ Galveston/ Beaumont/ Port Arthur
Wind Speed RMSE*	<2.0 m/s	1.2	1.3	1.3
Wind Speed Bias	± 0.5 m/s	0.0	0.5	0.4
Wind Speed IOA**	>0.60	0.68	0.81	0.63
Wind Direction Gross Error	<30 deg	36	23	30
Wind Direction Bias	± 10 deg	-6	-5	2
Temperature Gross Error	<2.0 K	2.1	1.3	1.5
Temperature Bias	± 0.5 K	-1.3	0.4	-0.6
Temperature IOA**	>0.80	0.92	0.92	0.95
Humidity Gross Error	<2.0 g/kg	1.4	2.4	1.1
Humidity Bias	± 1.0 g/kg	-0.3	-1.6	-0.3
Humidity IOA**	>0.60	0.47	0.53	0.61

\* RMSE: root mean square error

\*\*IOA: index of agreement

### Processing of MM5 Meteorological Fields for CAMx

Meteorological data from the Run5g simulation were used to generate the required three-dimensional gridded meteorological fields shown in table B-4 for the September 13-20, 1999 CAMx model. The MM5 output fields were translated to CAMx-ready inputs using ENVIRON's MM5CAMx translation software. This program performs several functions:

- Extracts wind, temperature, pressure, humidity, cloud, and rain fields from each MM5 grid that matches the corresponding CAMx grid;
- Performs mass-weighted vertical aggregation of data for CAMx layers that span multiple MM5 layers;
- Diagnoses fields of vertical diffusion coefficient (Kv), which are not directly output by MM5 (Kv was diagnosed using the O'Brien 1970 method);

<sup>7</sup> Emery, C.A., E. Tai, and G. McGaughey. 2003b. "Revised Meteorological Modeling of the September 13-20, 1999 Texas Ozone Episode – Final Report." Prepared for The Texas Joint Near Nonattainment Areas and Texas Commission on Environmental Quality, by ENVIRON International Corporation, 101 Rowland Way, Novato, CA 94945 and the University of Texas at Austin, Center for Energy and Environmental Resources, 10100 Burnet Road, MS R7100, Austin, TX 78758. 31 March 2003

<sup>8</sup> Value in red denotes statistics outside the benchmark.

Table B-4. Meteorological Data Requirements for CAMx.

CAMx Input Parameter	Description
Layer interface height (m)	3-D time-varying layer heights for the start and end of each hour
Winds (m/s)	3-D wind vectors (u,v) for the start and end of each hour
Temperature (K)	3-D temperature and 2-D gridded surface temperature for the start and end of each hour
Pressure (mb)	3-D pressure for the start and end of each hour
Vertical Diffusivity (m <sup>2</sup> /s)	3-D vertical exchange coefficients for each hour
Water Vapor (ppm)	3-D water vapor mixing ratio for each hour
Cloud Cover	3-D cloud cover for each hour
Rainfall Rate (in/hr)	2-D rainfall rate for each hour

The MM5CAMx program has been written to carefully preserve the consistency of the predicted wind, temperature, and pressure fields output by MM5. This is important for preparing mass-consistent inputs, and consequently, for obtaining high quality performance from CAMx.

Most data prepared by MM5CAMx were directly input to CAMx. A single 40-meter deep CAMx surface layer was extracted from aggregation of the lowest two 20-meter MM5 layers. The structures for vertical layers for MM5 and CAMx are shown in table B-5. The CAMx vertical layer structure is consistent with recommendations described in the EPA's 8-hour modeling guidance (EPA, 1999) which specifies that the surface layer should be no more than 50 meters deep, no layer beneath the mixing height should be greater than about 300 meters thick, 7-9 vertical layers with the planetary boundary layer and 1-2 layers above it. (Emery, C.A., et. al., 2002)

The horizontal extent of the MM5 4-km domain was defined to be much larger than the CAMx 4-km domain (the MM5 domain reached to the Texas-Louisiana border). The differences in spatial extents of the domains could lead to inconsistencies in the flow and hydrodynamic fields just inside and along the eastern boundary of the CAMx 4-km grid and 12-km grids, if meteorological fields for the 12-km CAMx grid were derived only from the 12-km MM5 output. To ensure consistency for this portion of the CAMx grids, an alternative approach was designed. The 4-km meteorological output fields were extracted for the entire MM5 4-km grid coverage using MM5CAMx, averaged to 12-km resolution, then used to replace the meteorological fields on that portion of the CAMx 12-km grid.

Table B-5. Vertical Layer Structure for MM5 and CAMx for Sept. 13-20, 1999 Episode

k	sigma	pressure	height	thickness	CAMx Layers
28	0.0000	50.00	18874.41	1706.76	
27	0.0250	73.75	17167.65	1362.47	
26	0.0500	97.50	15805.17	2133.42	
25	0.1000	145.00	13671.75	1664.35	
24	0.1500	192.50	12007.40	1376.75	
23	0.2000	240.00	10630.65	1180.35	
22	0.2500	287.50	9450.30	1036.79	
21	0.3000	335.00	8413.52	926.80	
20	0.3500	382.50	7486.72	839.57	
19	0.4000	430.00	6647.15	768.53	
18	0.4500	477.50	5878.62	709.45	
17	0.5000	525.00	5169.17	659.47	
16	0.5500	572.50	4509.70	616.58	
15	0.6000	620.00	<b>3893.12</b>	579.34	--12---
14	0.6500	667.50	3313.78	546.67	
13	0.7000	715.00	<b>2767.11</b>	517.77	--11---
12	0.7500	762.50	2249.35	491.99	
11	0.8000	810.00	<b>1757.36</b>	376.81	--10---
10	0.8400	848.00	<b>1380.55</b>	273.60	---9---
9	0.8700	876.50	<b>1106.95</b>	266.37	---8---
8	0.9000	905.00	<b>840.58</b>	259.54	---7---
7	0.9300	933.50	<b>581.04</b>	169.41	---6---
6	0.9500	952.50	<b>411.63</b>	166.65	---5---
5	0.9700	971.50	<b>244.98</b>	82.31	---4---
4	0.9800	981.00	<b>162.67</b>	65.38	---3---
3	0.9880	988.60	<b>97.29</b>	56.87	---2---
2	0.9950	995.25	<b>40.43</b>	20.23	---1---
1	0.9975	997.62	20.19	20.19	
0	1.0000	1000.00	0.00		=====Surface=====

An alternative set of vertical diffusivity input fields were developed for CAMx. Vertical diffusivities ( $K_v$ ) are important inputs to the CAMx model because they determine the rate and depth of mixing in the PBL and above. Original diffusivity fields derived by MM5CAMx were passed through an additional algorithm that sets minimum  $K_v$  values between layers 1 and 2 to ensure that nocturnal stability near the surface is not overstated. The minimum value is tied to the land use (e.g., urban, forest, agricultural, water, etc.) to represent different impacts of mechanical mixing and surface heat input (e.g., urban heat island effect).

References:

Emery, C.A, E. Tai., G.M. Wilson, and G. Yarwood. 2002. "Development of a Joint CAMx Photochemical Modeling Episode for the Four Southern Texsa Near Non-Attainment Area." Prepared for the Texas Near Non-Attainment Areas through the Alamo Area Council of Governments, by ENVIRON International Corporation, 101 Rowland Way, Novato, CA 94945. 3 April 2002.

Emery, C.A., E. Tai, and G. McGaughey. 2003. "Revised Meteorological Modeling of the September 13-20, 1999 Texas Ozone Episode – Final Report." Prepared for The Texas Joint Near Nonattainment Areas and Texas Commission on Environmental Quality, by ENVIRON International Corporation, 101 Rowland Way, Novato, CA 94945 and the University of Texas at Austin, Center for Energy and

Environmental Resources, 10100 Burnet Road, MS R7100, Austin, TX 78758. 31 March 2003

ENVIRON, UT/CEER 2003 presentation “Revised MM5 Modeling for the Texas Joint NNAs”, slide 50

United States Environmental Protection Agency (EPA), 1999. “Draft Guidance on the Use of Models and Other Analyses in Attainment Demonstrations for the 8-Hour Ozone NAAQS. EPA 454/R-99-004, U.S. Environmental Protection Agency, Research Triangle Park, NC. May 1999.