Attachment 2

Meteorological Modeling of the TexAQS 2000 Episode

August 25, 2000 - September 1, 2000

Background

Meteorological modeling is a prerequisite for photochemical air quality modeling, and TCEQ staff selected the Fifth Generation Meteorological Model (MM5) developed by the National Center for Atmospheric Research (NCAR) and Penn State University (PSU) for the TexAQS 2000 episode of August 25, 2000 - September 1, 2000. Professor John Nielsen-Gammon of Texas A&M University (TAMU) was chosen to perform the meteorological modeling in consultation with TCEQ staff. Dr. Nielsen-Gammon is the present Texas State Climatologist and was the primary forecaster for flight planning during the TexAQS 2000 campaign. In these roles, Dr. Nielsen-Gammon became especially well acquainted with this episode, and he was in an excellent position to extend his work running MM5 for forecasts to the running of MM5 in retrospective mode for use in SIP quality-modeling. TCEQ staff developed a set of primary objectives for this project and worked in conjunction with Dr. Nielsen-Gammon to develop a protocol by which this project would proceed.

TCEQ staff outlined the objectives for MM5 modeling during initial discussions with Dr. Nielsen-Gammon. The first objective was for MM5 to be run in the most realistic physical configuration so that performance was first evaluated by choice of physics options. Secondly, after MM5 had a well justified base configuration, the goal was to utilize as much of the TexAQS 2000 special study data as possible once consideration was made of which data were appropriate for data assimilation into the model, and which data were most useful for model validation. Third, in light of his familiarity with the daily variations in this episode's weather, Dr. Nielsen-Gammon was given wide latitude to evaluate those features which were, in his opinion, of greatest importance. Finally, the process of model evaluation was to take place iteratively so that TCEQ staff could, in consultation with Dr. Nielsen-Gammon, weigh which would be the most productive routes for continuing work.

The following reports provide a summary of the work conducted by Dr. Nielsen-Gammon during the project period extending from August 31, 2001 through August 31, 2002. Each of these reports is available from the TAMU website http://www.met.tamu.edu/results or from the TCEQ website http://www.tnrcc.state.tx.us/air/aqp/airquality_contracts.html#section3. The first report, which is Attachment 3-1, is entitled *Initial Modeling of the August 2000 Houston-Galveston Ozone Episode*, December 2001. This document introduces the episode and has an initial discussion of the daily variations in meteorology that need to be modeled correctly. Also included in this document is the basic MM5 configuration and a preliminary assessment of how the model results are dependent on the model configuration. The second report, which is Attachment 3-2, is the *Evaluation and Comparison of Preliminary Meteorological Modeling for the August 2000 Houston-Galveston Ozone Episode*, February 5, 2002. Data from TexAQS 2000 did not begin to become available until the fall of 2001. This report summarizes the status of the special study data that were utilized in an intermediate series of model runs. Along with this data review, a further discussion of daily weather variations was included so that meteorological features which were looked at as part of model performance evaluation could be introduced. The last part of this report evaluated temperature biases, location of precipitation, development of the planetary boundary layer (PBL), and winds with modeling performed to date. The third report in this series, which is Attachment 3-3, is *Meteorological Modeling for the August 2000 Houston-Galveston Ozone Episode: PBL Characteristics, Nudging Procedure, and Performance Evaluation*, February 28,

2002. This report described in detail the ability of the MM5 model to capture those physical features which Dr. Nielsen-Gammon considered most relevant to the TexAQS episode. The first of two statistical summaries summarized the performance of the MM5 configuration in February 2002 and various model changes that were evaluated while photochemical modeling was getting started. This statistical summary, Attachment 3-4, is entitled *Meteorological Modeling for the August 2000 Houston-Galveston Ozone Episode: METSTAT Statistical and Model Runs from March-June 2002*, *June 21, 2002*. A second statistical report re-evaluated the MM5 modeling statistics after a time bias was discovered in the observational nudging, and also evaluated model improvements made during the summer of 2002. This last report is the *Meteorological Modeling for the August 2000 Houston-Galveston Ozone Episode: Improved Data Assimilation and Statistical Evaluation*, *August 29, 2002*. In the following sections of this Attachment we will refer to the above documents as NG01, NG02a, NG02b, NG02c, and NG02d, respectively.

Since a thorough exposition is available in the documents described above, the purpose of this document is to highlight important conclusions of each report. The following sections will center around important modeling issues raised by either commission staff or Dr. Nielsen-Gammon, will present the rationale for choices in either model configuration or use of data which impacted the particular modeling issue, and will explain which indicators were used to evaluate model performance in either the base case or one of its variations.

Key Points from Report NG01

- Dr. Nielsen-Gammon characterized the evolution of the TexAQS 2000 episode broadly into two regimes. He noted that in all cases where convection was absent, the observed winds were sensitive both to the cyclic diurnal winds and large-scale, or synoptic winds. The localized Galveston Bay breeze is separate and modifies the observed wind further. As per discussion and figures from the report NG01, hourly winds were averaged across several days at a time so that a discontinuity of meteorological features became apparent after August 29. During the first regime extending from August 25 through August 29, there was very little vertical shear throughout twenty-four hour periods, which indicated good mixing in the PBL.

- Between August 30 and September 1st, various components of the atmospheric forcing combined to create different atmospheric behavior. Observed winds indicated an adverse shear. A strong inversion and low level jet were present during evening hours. A detailed description of this mechanism is in section 2d of report NG01.

- MM5 has long been recognized to be sensitive to available soil moisture; therefore, a decision to modify the default value must be carefully supported. Dr. Nielsen-Gammon's important work in adjusting soil moisture availability is documented in Table 3 of report NG01.

- Several possible interactions between available soil moisture and two PBL options are summarized in Table 4 of report NG01. The two PBL options under evaluation were called "MRF" and "Gayno-Seaman". Among the conclusions drawn from the first series of MM5 model runs was that modeled surface temperatures alone would not be sufficient to distinguish performance between the two different PBL schemes. Table 6 of the report NG01 shows that temperature biases were not systematic between different days and different sites.

- In addition to comparisons of surface temperatures and winds, MM5 was validated against GPS-sonde and rawinsode soundings of the lower atmosphere. After averaged modeled temperatures and dewpoint between 920 millibars and 960 millibars (within the well-mixed daytime PBL) were compared to the averaged sounding data, Dr. Nielsen-Gammon concluded that it was appropriate to reduce available soil moisture through the episode. This comparison of model data to sounding data is presented in Table 7 of report NG01. Changes to MM5 code reflecting these changes were reported in NG02b.

Key Points from Report NG02a

- Dr. Nielsen-Gammon addressed particular model validation issues in his preliminary report NG01. In addition to the use of surface temperatures and sounding data discussed above, Dr. Nielsen-Gammon also considered the amount of modeled convective activity as part of his model analysis in reports NG01 and NG02a..

- The use of *analysis* nudging was tested on either the 36-kilometer grid alone or on both 36- and 12-kilometer grids. MM5 wind fields were nudged towards the same global EDAS analyses used to initialize MM5 and provide its boundary conditions. It is generally presumed that the primary benefit of nudging is to correct the possible drift of the large scale winds calculated by MM5 from the fields used for initialization and boundary conditions. One of the benefits noted by Dr. Nielsen-Gammon (NG01) from nudging on both 36- and 12-kilometer grids was improved modeling of convective activity.

- In this report, the choice of PBL scheme was also found to have an impact on predicted cloud formation and model precipitation. The lower PBL calculated with Gayno-Seaman increased the concentration of moisture aloft and was found to produce a super-adiabatic layer. These features contributed a strong wet bias. One of the benefits noted in NG02a is that corrections to available soil moisture availability minimized what would otherwise have been a bias in surface temperatures.

Key Points of NG02b

- Dr. Nielsen-Gammon ran MM5 in different configurations during the spring of 2002 in order to continue investigation of the strength of the nocturnal inversion and nocturnal jet which were important features of regime two (August 30 through September 1st). He also evaluated the timing of the sea breeze, the strength of the inversion over the sea breeze, and observed depth of the PBL as a means of testing the dependence of PBL algorithms on new model configurations.

- MM5 code was modified to allow available soil moisture to be corrected daily. In the preliminary model runs, this correction was not incorporated, and so temperature biases did not reflect the full diurnal swing of surface temperatures. Once these corrections were incorporated, modeled surface temperatures matched observational data quite well.

- Two MM5 sensitivity runs included increasing the number of vertical layers and reducing the amount of diffusion between the top of the PBL and the free atmosphere in the MRF scheme. The first change was intended to better resolve the nocturnal inversions occurring during second half of the episode. The latter change was intended to test whether the current MRF scheme was causing so much mixing of momentum that the nocturnal inversion and the capping inversion above the sea breeze were suppressed. Neither sensitivity improved model performance.

- Day time performance of MRF was considered better than Gayno-Seaman despite the fact that MRF tended to over predict the PBL by approximately 30%. The decision to use the MRF algorithm was based upon the conclusion that the photochemical model would require the best possible day time performance.

- Validation of profiler data was a joint project involving Dr. Nielsen-Gammon and both NOAA's Aeronomy Laboratory and Environmental Technology Laboratory. Once this data was quality assured, Dr. Nielsen-Gammon utilized the data for *observational* nudging. Observation nudging uses specific special study data at particular points. A 150 kilometer horizontal radius of influence for each profiler was selected. In contrast, the analysis nudging discussed in NG01 utilized EDAS wind fields which had data for each point in the domain.

- The final run prior to February 28 incorporated the best determined physical configuration and utilized the profiler data for observational nudging. Several figures report on the improved statistical performance for domain winds. Section 6b of NG02b indicates RMS errors between 1.3 and 1.8 meters/second which improve with height. None of the model runs without nudging had RMS errors less than 2 meters/second. Biases tended to be less than 0.3 meters/second below 2500 meters. This model configuration was subsequently identified as the "driver" run - this label referred to the use of the MM5 model output to "drive" the meteorology in photochemical modeling.

- The strong nocturnal inversion and jet that were observed in during regime two of the episode were not well represented by the MM5 driver run.

- In the comparisons of the MM5 driver winds to surface observations on each episode day, both successes and room for improvement were noted. On August 25 the second highest value of peak ozone was measured, but MM5 winds did not reflect the northeasterly flow reported by surface observations late in the afternoon. On the other hand, August 30 was the day on which the episode's highest ozone was reported, and on this particular day, MM5 day time winds were judged by Dr. Nielsen-Gammon to be very good.

Key points from NG02c

- Soil moisture corrections necessary for the 4-km grid were removed from the 12- and 36-km grids, since the drought over east-central Texas was not as significant over a larger regional area. This factor had very little impact on model results or statistics.

- Modeled upper level moisture was artificially reduced to suppress the convective activity on August 31 and September 1 which was developing ahead of observations along the eastern portion of the 4-kilometer grid.

- MM5 was run with observational profiler nudging that utilized a shorter time window for data assimilation. This shorter assimilation window was to investigate whether profiler data could strengthen the land-sea breeze. In addition, the profiler data set combined the best of two different NOAA data sets. The statistical metrics for this run were virtually identical to the initial driver run.

- METSTAT, the model performance evaluation package, extrapolates calculated variables such as winds and temperature to heights were observations are available. Dr. Nielsen-Gammon identified an error in the implementation of the vertical interpolation scheme used by METSTAT. The nighttime interpolation scheme of METSTAT effectively assumes a neutral stratification of the environment rather than a more probable stable stratification. The effect of this error would be to calculate a higher bias in wind speeds at night than was actually the case.

Key points from NG02d

- In this report, Dr. Nielsen-Gammon provided a detailed explanation of the corrections needed for the vertical interpolation of modeled variables in the METSTAT program. The original ENVIRON program had assumed a constant bulk Richardson number throughout the PBL. Instead, Dr. Nielsen-Gammon assumed a constant Monin-Obukov length and then described the new procedure for calculating vertical interpolation of variables. This change lowered hourly wind biases, especially in the first part of the episode. Temperature statistics also improved. The changes made by Dr. Nielsen-Gammon to the

  METSTAT program provide a more accurate representation of MM5 performance. The new version of METSTAT was also applied to the new MM5 runs described below.

- An important change in MM5 model setup was identified when Doppler lidar data was being prepared for data assimilation on the August 25 episode day. When Dr. Nielsen-Gammon first prepared the profiler data for observational nudging, he reformatted the Julian date format used with the profiler data to the Greenwich Mean Time format used in MM5, and he simultaneously interpolated data from the whole hour to half-hour. The intention was to provide nudging at the mid-point of the hourly interval that is output from MM5. Instead, the data were inadvertently assigned to a time 1.438 hours *after* the midpoint intended for nudging. After a correction was made, the associated statistics changed on all days, but August 25th was the most improved day of the episode once the appropriate nudging was performed. Since this day had the second largest peak in the episode, this was considered an important improvement.

- In NG02b, Dr. Nielsen-Gammon conjectured that the inability of MM5 to capture the northeasterly component found among surface winds on the morning of August 25 was due to the fact that the MM5 was nudged to profiler data which had a southwesterly component at 200 meters. Once the Doppler lidar was quality assured for August 25th, the data from the lidar, which were valid between the surface and 200 meters, were used for observational nudging in a new model run. The statistics from the new run show a small improvement on the 25th, but even more importantly, the wind fields show a much improved organization at the lowest levels in during the morning hours.

Meteorological Post-Processing

The performance of CAMx modeling is described in another attachment. However, a few additional comments about the input of meteorological fields that were prepared for CAMx are warranted at this point.

The reports provided by Dr. Nielsen-Gammon carefully examined various options for MM5 model configuration to best reflect the conditions of the Houston-Galveston environment during August 25th through September 1, 2000 (termed the "driver" configuration). The preparation of meteorological fields for the CAMx model required post-processing by a program called MM5CAMx written by ENVIRON. Horizontal interpolation of MM5 variables was unnecessary since the MM5 grid and CAMx utilized the same Lambert-Conformal projection. Vertical interpolation was minimized by defining matching sigma levels in the lowest ten layers. The details of the MM5 and CAMx grid definition have been summarized in the modeling protocol.

For the purposes of air quality modeling, the extent of vertical mixing is of great importance. Using the MRF parameterization scheme, which was part of the MM5 driver configuration developed by Dr. Nielsen-Gammon, a predicted planetary boundary layer (PBL) height is calculated by MM5. The alternative Gayno-Seaman PBL parameterization calculated turbulent kinetic energy (TKE) as well. The post-processing program MM5CAMx does the required interpolation of meteorological variables from MM5 to CAMx grids, and equally importantly, uses information about PBL height or TKE to calculate the vertical diffusivities needed by CAMx.

Since the vertical diffusivities calculated by MM5CAMx significantly affected the performance of CAMx, two significant adjustments to the MM5-predicted PBL heights were made prior to running the post-processor. First, for reasons discussed in NG01 and NG02c, the MM5 PBL heights were scaled to 70% of the MM5 values prior to the calculation of the vertical diffusivities in the primary CAMx runs. The choice of 70% was based upon an analysis of rawinsonde data on August 30th, which was the peak day during this episode. Secondly, for purposes of evaluating CAMx sensitivity to the vertical diffusivities, other CAMx runs utilized vertical diffusivities prepared from PBL heights based upon observed profiler data on each day of the episode.

To work toward further improvement in the representation of PBLs, hourly averaged observed

PBL heights were calculated from the profiler network. Hourly predicted MM5 PBL heights were also averaged at the same grid cells where each profiler was located. A ratio of hourly averaged observed PBL heights to hourly averaged predicted PBL heights was used to scale the MM5 PBL heights at all other grid cells on an hour by hour basis. The resultant PBL heights had a two-dimensional structure which was predicted by MM5, but adjusted up or down according the hourly calculated ratio. These scaled PBL heights were then used as input to the MM5CAMx post-processor.

The evaluation of the CAMx runs indicates that higher ozone resulted from the scaling of the predicted PBL by 70% than by the scaling of the MM5 PBL to average profiler observations. The summary of ozone statistics and other performance metrics are available in Attachment 6, Performance Evaluation. TCEQ staff believe that adjustments based upon available data from rawinsonde or profiler data are credible, and discussions with Dr. Nielsen-Gammon support the conclusion that they are reasonable. The use of profiler data for PBL adjustment is currently a sensitivity analysis which will be pursued further in future modeling.

Conclusions

The MM5 modeling summarized here and discussed in greater detail in the reports NG01, NG02a, NG02b, NG02c, and NG02d involved an iterative process to identify the most important physical features of August 25 through September 1st, 2000 and to evaluate model configurations which best reflected the reality of the TexAQS 2000 episode. Consideration of important parameters such as available soil moisture, and information about the vertical structure of the atmosphere from radiosonde, GPS sonde, and profilers helped define the most appropriate physical configuration of MM5. Only after several sensitivities were complete was observational nudging used to refine MM5 and generate output with the best overall performance. The important additional work described in NG02c and NG02d included important additional work which included corrections to profiler data and the inclusion of doppler lidar for observational nudging.

The adjustments made to PBL height during post-processing were made to investigate the dependence of CAMx upon calculated vertical diffusivities. As much as possible, the adjustments were designed to reflect real data when observations of PBL were available. The first adjustment, scaling the PBL heights to 70% of the predicted MM5 values, was based upon an analysis of rawinsonde data on the peak episode day. The CAMx runs analyzed in Attachment 6, Performance Evaluation, relied upon this particular adjustment. The use of alternate meteorological data from radar profilers to modify the PBL heights has a different impact on CAMx model performance, and will be part of future work.