Validation of Physical Processes in MM5 for Photochemical Model Input: The Houston 2000 Ozone Episode

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1. INTRODUCTION

In work funded by the Texas Natural Resource Conservation Commission, we have been asked to produce MM5 simulations of the August 25-September 1 2000 ozone episode in the Houston-Galveston area. Most meteorological model runs for photochemistry purposes are validated with data from a handful of surface sites and perhaps a rawinsonde launch site. This episode occurred during the TexAQS-2000 field program, and special meteorological observations include three radiosonde launch sites, six wind profilers, a Doppler Lidar, four instrumented aircraft, and special surface flux measurements. The wealth of observations enabled an unusually comprehensive analysis of the physical processes leading to high ozone in the Houston area, and also permitted a physically-based model validation effort.

2. AIR POLLUTION METEOROLOGY IN THE HOUSTON AREA

During the TexAQS-2000 field program, wind patterns in Houston were dominated by the diurnal wind cycle associated with the sea breeze. As we have reported elsewhere, this diurnal cycle is peculiarly enhanced by the near-resonance between the diurnal frequency and the inertial frequency at the latitude of Houston. In addition to the "traditional" sea breeze front, which forms during late morning along the coastline and progresses inland during the afternoon while being modulated by the ambient wind, there is a larger-scale diurnal-inertial oscillation which extends throughout the boundary layer. This larger-scale response takes the form of a clockwise rotation of the wind superimposed on the ambient flow, with maximum onshore component after sunset. This regular oscillation is suppressed at night at the surface, but is readily observed with profilers and offshore buoys, even several hundred km from the coastline.

During the latter half of the ozone episode, a shore-parallel low-level jet developed repeatedly at night and reached its maximum strength around sunrise. This jet appears to have been caused by frictional decoupling in the presence of adverse low-level shear and was positively reinforced by the clockwise rotation of the wind associated with the diurnal forcing. The low-level jet reached observed speeds of 15 m/s at a height of 300-400 m above the ground.

High levels of ozone occurred in Houston when the amplitude of the diurnal wind oscillation (~3.5 m/s) was almost exactly matched by the large-scale wind speed around the Bermuda

high. Under such circumstances, the wind stagnates at those hours when the diurnal rotation cancels the large-scale wind; for large-scale southeast winds, this stagnation occurs during late morning. High concentrations of ozone precursors build up in the planetary boundary layer (PBL), and high levels of ozone are observed a few hours later. Additional factors in Houston ozone include PBL depth and the possible stagnation of shallow layers of pollutants over Galveston Bay.

3. MODEL VALIDATION STRATEGY

The large number of special observations permits the use of four-dimensional data assimilation (FDDA) to improve the simulation. However, the observations are insufficient to resolve circulations along a complex coastline such as that of Galveston Bay. Therefore, model validation has focused on the improving the ability of MM5 to simulate the local-scale winds driven by topography, hopefully minimizing aliasing of small-scale model errors onto a larger scale during FDDA. The strategy involves three processes: diurnal heating, wind evolution, and FDDA. These processes are in addition to conventional validation strategies, such as statistical scores and examination of model output fields for reasonableness.

a) Diurnal Heating

Diurnal heating validation was an essential first step because the simulated local-scale circulations are driven by the heating contrast across the coastline or across land use boundaries. The strength of the circulation depends on the diurnal amplitude of the temperature difference: how much the temperature difference changes from day to night. The most direct measure of this physical process is the error in simulating the difference between maximum and minimum temperatures within the PBL.

Observations are not quite adequate to examine this aspect of the simulation. Surface observations provide information on the diurnal temperature cycle near the ground, but nighttime surface temperatures were found to be very sensitive to land use variations, which strongly controlled the strength of the nocturnal inversion. Station-to-station variability was much larger in the observations than in the model simulations, and model biases in the minimum temperatures ranged from –1 C to +3 C. Maximum temperatures were more uniform, and biases were generally less than +/- 1 C. This level of accuracy was obtained with the use of the MRF PBL scheme and reduction in soil moisture availability in the Houston area to account for drought conditions. For the final simulations for photochemical modeling, the MM5 code was modified slightly to allow for the soil moisture availability to be modified during restarts.

Soundings proved to be a second critical source of information. There were no enough soundings and dates in the episode to reliably estimate the amplitude of the diurnal temperature cycle as a function of altitude, but the soundings were useful for checking the daytime PBL depth (a measure of the amount of heating the atmosphere has undergone) and for spot-checking nighttime temperature errors. We confirmed that the nighttime temperature errors were due to an underestimate of the strength of the nocturnal temperature inversion in the lowest 100-200 m of the atmosphere. Because these errors were shallow, they would not significantly

affect the diurnal wind cycle. Orography in the Houston area is too flat to allow drainage winds or significant classical land breezes to develop.

b) Diurnal Wind Response

Once the MM5 had been set up to successfully simulate the diurnal heating cycle, the next step was a check of the winds produced by the MM5 in response to the diurnal heating cycle. In the physical validation of temperatures described above, we chose not to use overall measures of temperature performance such as bias and RMS error. Similarly, overall measures of wind performance are inappropriate for addressing the more focused issue of the model performance in simulating the diurnal variation of the winds.

To perform this validation, a 24-hour running mean was applied to the wind profiler data, following quality control for bird contamination and other anomalies by Allen White and David White of NOAA/ETL. A similar 24-hour running mean was applied to the model output. Performance statistics were computed separately on the errors of the 24-hour running mean and on the errors of the departures from the 24-hour running mean. Time series and time-height sections were plotted and examined. Although this level of rigor was not necessary, it would also have been possible to extract the amplitude and phase of the diurnal cycle from the observations and model simulation and compute amplitude and phase errors.

We found that the MM5 did well in recreating the amplitude of the diurnal cycle during the first half of the ozone episode. The vertical structure of the diurnal wind response in the MM5 was deficient, in that it failed to show the observed sustained nighttime wind speeds and the upward phase propagation of the diurnal signal. The cause of these errors is not known.

During the second half of the ozone episode, when a low-level jet was present, the MM5 performed poorly. The poor performance is not surprising, since the low-level jet is produced by a complex interaction between the diurnal variations of heating and turbulence. Typically, the model would underestimate the strength of the low-level jet and would cause it to rotate clockwise too far. The performance of the Gayno-Seaman scheme was somewhat better than that of the MRF scheme. Based on the premise that the error in the MRF scheme was caused by too-large vertical diffusion of momentum in the free atmosphere, the MRF scheme was altered to correspond more closely to the originally-coded scheme, with a reduction by about one order of magnitude in the vertical mixing coefficient. The simulation of the low-level jet improved, but the overall wind performance was slightly degraded so this model modification was abandoned.

Another relevant aspect of the diurnal wind response was the timing and vertical structure of the sea breeze front. For this aspect of model performance, the accuracy of the simulations was estimated subjectively by comparison with the profiler and radiosonde data. As with the low-level jet, neither scheme performed especially well. The MRF scheme was too weak with the temperature difference between the sea breeze air and the continental air. The Gayno-Seaman scheme, on the other hand, was too strong, producing much to strong an inversion atop the advancing marine air where the MRF scheme had failed to produce any inversion at all.

c) Four-Dimensional Data Assimilation

Requirements for accuracy of MM5 simulations are especially rigorous for photochemical applications. A systematic wind error of 1 m/s over six hours produces a trajectory displacement error of 21.6 km and can mean the difference between a successful and unsuccessful simulation.

As noted earlier, observations were insufficient to resolve local-scale circulations, but they were perfectly adequate for representing the large-scale wind field. Furthermore, the diurnal wind response was found to have deficiencies that the FDDA scheme should also attempt to correct. Meanwhile, the smaller-scale and high-frequency wind variations in the observations should not be assimilated into the model.

To accomplish these goals, the nudging of the profiler data was performed with a horizontal radius of influence of 150-200 km and a time window of 2-4 hours. Statistical tests such as those described in section 3b showed that this nudging reduced the error in the 24-hour mean winds to much less than 1 m/s, while reducing the total RMS wind error to around 1.5 m/s from its previous level of 2.5-3.0 m/s. This work is still underway; the Doppler Lidar wind profiles are yet to be incorporated, and data withholding experiments must be conducted to estimate the true improvement in model accuracy.

4. SUMMARY

Although not described here, standard statistical measures of performance have been applied to the final model run, including FDDA. These measures are useful indicators of overall model performance, but would not have been useful in assessing the model's ability to simulate critical physical processes. The physical validation was necessary to identify model deficiencies, develop and test improvements that could compensate for those deficiencies, and minimize possible negative impacts on the simulation caused by immediate use of four-dimensional data assimilation.

More complete discussions of the model validation and model performance are found in a set of three reports available from TNRCC and from <http://www.met.tamu.edu/results>.