10.24 RESULTS FROM THE NOAA, FSL PHOTOCHEMICAL FORECAST MODEL: COMPARISONS TO AIRCRAFT AND SURFACE DATA DURING TEXAQS-2000

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1. INTRODUCTION

The photochemical and meteorological data collected during the TEXAQS-2000 field study provide valuable information regarding O_3 production and transport in the Houston-Galveston region. Aircraft and surface observations of O_3 and its precursors are able to distinguish photochemical O_3 production rates and efficiencies from individual sources such as petrochemical and power generating facilities, and also from more widespread regions such as the Houston urban core, petrochemical complexes and shipping channels that extend from Houston east and south along the Galveston Bay. Preliminary analysis also suggests that the location and magnitude of high O_3 levels (120-250 ppbv) observed near Houston depends on synoptic conditions that are determined by interactions between large scale meteorological forcing and smaller scale, boundary layer processes such as land and sea breeze dynamics that are unique to this coastal/bay location.

Aside from the significant scientific and policy implications of the TEXAQS-2000 field observations, the experiment also provides a unique opportunity for diagnosing state-of-the-art photochemical forecast models. Fundamental uncertainties are associated with these models, which include but are not limited to the proper model resolution, data assimilation strategies, the adequacy of emissions, photochemical mechanisms, and the many physical parameterizations on which they depend. Since these models are often used for policy guidance (e.g. O_3 control strategies), it is important that their deficiencies and biases are at least characterized, and hopefully eliminated, through proper comparisons with observations. This work presents preliminary findings from the comparison of results from one such model with the observations collected during TEXAQS-2000.

2. NUMERICAL MODEL

Details of the FSL photochemical forecast model are given in Grell et al. (2002, this issue). Briefly, the Penn State/NCAR Mesoscale Model (MM5, version 3) is modified to include the Regional Acid Deposition Model version 2 (RADM2) gas-phase photochemical mechanism of Stockwell et al. (1990). An important and unique feature of this model is the "on line" calculation of photochemical species with the same transport processes and time step used in the meteorological calculations. The model is run in a nested configuration for 4 distinct domains: from a 60km resolution covering almost the entire continental U.S. to a 1.67km domain covering southeast Texas and western Louisiana. Emissions of O_3 precursors are taken from the U.S. EPA inventories for a typical summertime weekday (NET-96), and additional information provided by the Texas Natural Resources Conservation Center (TNRCC). The large number of prognostic variables and the requirement of timely forecasts necessitate the coding and implementation of the model on a distributed memory parallel computer platform.

3. PRELIMINARY RESULTS

During the summer of 2000 the model was run in real time in support of the TEXAQS-2000 field study. The model results presented here are from the forecasts calculated during the field study, although the use of the model in a post-analysis mode that includes more detailed emissions information is currently underway. The comparison of model forecast meteorological variables with observations is described in Bao et al. (2002, this issue). Results from the 1.67 km model domain are able to capture observed features of the land-sea breeze circulation that are important to the transport and fate of the species involved in O_3 photochemistry. The focus here is on comparisons of important photochemical quantities and relationships, and examples are shown for a very limited subset of the observed and model data.

Data collected on the afternoon of 8/30/00 from the NCAR Electra (250 - 720 m, AGL) in the region bounded by 29.3 to 29.9º latitude and 95.2 to 94.7º W. longitude are shown in Figures 1a,b in comparison to the model results. This was a cloud free day with large O_3 exceedances observed at several surface monitoring sites. The region covers a broad area over the shipping channels and various industrial sources along the western side of the Galveston Bay. Figure 1a shows that model O_3 is severely underpredicted, and the observed O_3-NOy relationship is not captured. Figure 1b shows tighter correlations between O_3+NO_2 versus the difference between NOy and NOx. Together, these figures suggest the model is too slow in converting NO from primary emissions into NO_2 and more oxidized nitrogen species such as HNO_3 and PAN. The slopes of the correlations in Figure 1b are a

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measure of oxidant production efficiency (Trainer et al., 1993), which is significantly less for the model. The non-methane hydrocarbon to NOx emission ratios from the emissions inventory are typically an order of magnitude less than what was observed d o w n w i n d o f

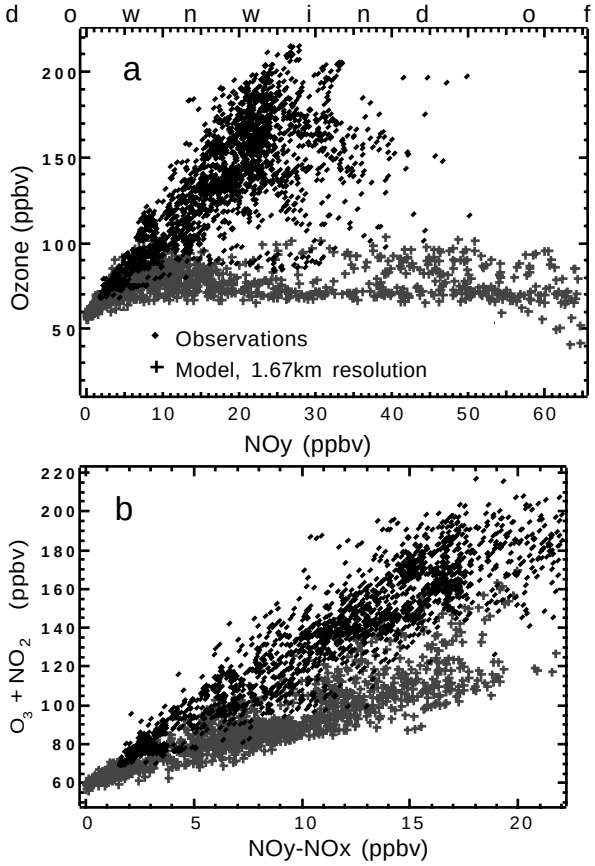

Figure 1. Observations and model correlations of O_3 versus NOy (a), and O_3+NO_2 versus NOy minus NOx (b) for the ship channel region on 8/30/00.

industrial sources during TEXAQS-2000, particularly for the light alkenes; ethylene and propylene. The speed and efficiency of oxidant production is known to be extremely sensitive to NMHC/NOX emission ratios for the high NOx regimes encountered during the study (McKeen et al., 1991). Thus, a systematic underestimation of propylene and ethylene emissions is a likely cause of the discrepancies.

Figure 2 shows the comparison between model and observed O_3 at the intensive surface measurement site located at LaPorte. This site is within the industrial and shipping corridor near the Galveston Bay. While the model reproduces well the diurnal cycle and peak concentrations from 8/26/00 through 8/29/00, it fails to predict the high O_3 levels observed on 8/25 and 8/30. Wind patterns on 8/30/00 (not shown) are light with local recirculation, while the other days do not. Moreover, the model consistently underpredicts surface O_3 at other monitoring sites well downwind of the industrial and shipping corridor. These results again suggest the model is unable to simulate the rapid and efficient production of O_3 from particular industrial sources, but may do a reasonable job for urban emissions and when larger scale forcing of O_3 is relatively more important.

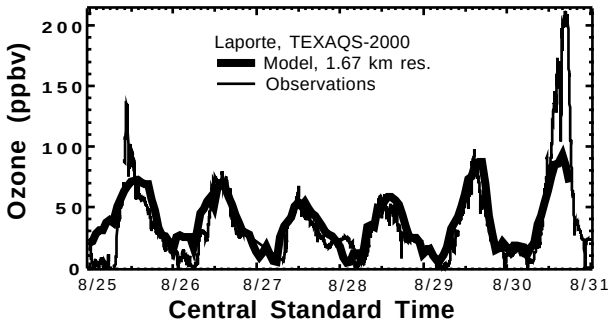

Figure 2. Observed and model O_3 at LaPorte, TX.

4. CONCLUDING REMARKS

The results presented here provide a glimpse of the photochemical comparisons between the NOAA/FSL photochemical forecast model and data collected during TEXAQS-2000. In its original configuration the model is systematically unable to predict the high levels of O_3 often encountered aloft and on the ground. Comparisons of NMHC/NOy ratios strongly suggest the emissions of NMHC, particularly ethylene and propylene, are too low in the model. Modifications to the emissions inventory are needed to reflect this discrepancy, as well as a reanalysis of the model results with modified emissions included. It is anticipated that several iterations of the forecast model will be necessary in order to explain not only observed O_3 levels, but also the levels of many secondary intermediates also measured during the study.

5. REFERENCES

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