SENSITIVITY OF CMAQ TO THE SCALING OF NITROGEN EMISSIONS

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1. INTRODUCTION

Because emission reductions are a key component of air quality planning, the sensitivity of the regional models to emissions is of great interest. A general framework for interpreting emission sensitivity is provided by Dennis et al., (1999), who emphasized the importance of considering the model's response surface in explaining and predicting how perturbation to the inputs of the model influence outputs. In a similar vein, Clapp and Jenkin, (2001) differentiated between NOx-independent and NOx-dependent ozone production events based on Ox/NOx ratios in the local environment. Arnold et al. (Arnold et al., 2003) confirmed that CMAQ (Byun and Ching, 1999) is able to adequately capture these and other metrics indicative of different VOC/NOX sensitivity regimes. Other CMAQ emission sensitivity studies include several related to biogenic emissions, (Bell and Ellis, 2004; Poissant, 2000; Pressley et al., 2004; Yin et al., 2004). The sensitivity of CMAQ's prototype, MAQSIP to VOC was explored by Hakami et al. (Hakami et al., 2004) using direct sensitivity techniques.

The atmospheric modeling group associated with the Connecticut River Airshed/Watershed project (http://www.crawc.org/) is focusing on the factors affecting air quality and atmospheric deposition in the Connecticut River Basin. The study reported here is based on some preliminary work on the sensitivity of the basin's air to various types of local and remote emission sources. Specifically, we report on the sensitivity of O3, NO2 and NO to reductions in nitrogen emissions.

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2.0 METHODS

The hardware and software configuration used in this work was described in a benchmark study reported on in Bresnahan (Bresnahan et al., 2003). The May 2003 release of CMAQ (version 4.2.2) and other Models3 tools were compiled and used for this test. The spatial domain was based on a July 1997 MM5 run provided to us through NYDEC, that was generated at the University of Maryland. This dataset is based on the 36km Unified Grid and covers the eastern portion of the United States (67x78x21, 84Hrs).

Emissions were generated using SMOKE with the Net96 inventory. To generate scaled emissions, SMOKE was run using all area sources. The resulting output file was then run through a custom program that reduced nitrogen emissions for all grid cells and timesteps to 95, 90, 80 or 60 percent of their original values.

The sensitivity index used is: ***SI = (% change in metric) / (% change in emissions).*** This value is positive when a reduction in emissions causes a reduction in the metric, and negative when a reduction in emissions causes an increase in the metric. Values equal to 1 show that the percent change in both the metric and the emissions are equal. Two metrics were studied: the mean of the surface layer values, and the maximum of the surface layer values, for each of the 84 timesteps.

Because the spatial domain in this study consisted of 5226 grid cells, each of the surface layer means and maxima was calculated using 5226 values. The error bars for these means are extremely tight, and were left off of the graphs for clarity. Also, for clarity, the graphs of the means and maxima were plotted as curves, rather than as 84 separate points.

3.0 RESULTS AND DISCUSSION

The time series of the surface layer means for O3, NO2 and NO are shown in Figures 1 – 3, along with the associated values of the sensitivity index. The surface layer means of all three species exhibited diurnal cycling, and all three showed a reduction in magnitude with reduced nitrogen emissions. The sensitivity of the means to the scaling of emissions also exhibited diurnal variation with ozone and NO2 being most sensitive in the early afternoon, and NO most sensitive in the evening hours. Overall, the ozone mean showed the least sensitivity, and the NO mean the most sensitivity to emission reductions.

The time series of the maximum observed value in the surface layer for O3, NO2 and NO are shown in Figures 4 – 6 below, along with the associated values of the sensitivity index. All three species maxima showed diurnal variation, as did the sensitivity of the maximum values to nitrogen emission reductions, although the curves were not as smooth as those of the means. The species also differed in their degree of sensitivity: maximum NO was highly sensitive to emissions, NO2 somewhat sensitive, and O3 slightly sensitive. The maximum O3 values actually increased for a few timesteps in response to reduction in nitrogen emissions, particularly in the early afternoon hours.

While NOx was not calculated from individual grid cell observations, some general conclusions about the O3/NOx sensitivity regime in this scenario can be inferred from the means and maximum values of the component species reported here.

An estimate of mean suface layer NOx can be given by:

Est NOx = mean(NO2) + mean(NO)

A plot of this estimate for each of the timesteps, using unscaled emissions, along with the associated O3 value (not given here) shows that estimated NOx ranges from about 0.5 to 3.5 ppbV, with corresponding O3 from about 30 to 50 ppbV. This range of values corresponds to the “NOx independent” zone reported by Clapp and Jenkin (Clapp and Jenkin, 2001), which they describe as normally associated with regional sources rather than local emissions sources. This would make sense for our emission situation when we are considering only the surface layer mean.

When the range of maximum NO2 and NO values is examined, however, we see that both could get as high as 80 ppbV, making it at least conceivable that at individual grid cells NOx values potentially as high as 160 ppbV might be observed. This potential range of NOx crosses the ridgeline observed by Dennis et al. for peak O3, meaning that for at least some grid cells, a reduction in NOx (that produced by reducing nitrogen emissions) could potentially lead to an increase in O3 for that cell. This would explain the increase in maximum O3 that we observed in this study for some timesteps.

4.0 CONCLUSIONS

For O3, NO2 and NO, both the surface layer mean and the maximum value in the surface layer are sensitive to reductions in nitrogen emissions, however, ozone is much less sensitive, overall, than the other species. These metrics respond nonlinearly to emission reductions, and the degree of sensitivity shows a pronounced diurnal variation. When only the surface layer means are considered, this scenario seems to correspond to the NOx-insensitive regime described by Clapp and Jenkins (Clapp and Jenkin, 2001) In some situations, however, maximum O3 in the surface layer was shown to increase as nitrogen emissions are reduced, a factor which can be explained by the location of these species values with respect to the O3 response surface described by Dennis et al. (Dennis et al., 1999). .

7.0 ACKNOWLEDGEMENTS

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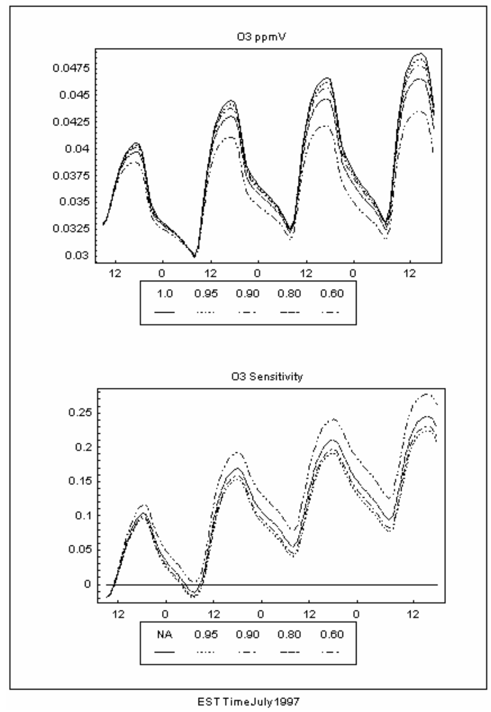

Fig. 1 Time series plots of surface layer mean ozone concentration, and sensitivity of that mean to scaling of nitrogen emissions. (1.0 is full, 0.60 is 60% of full emissions).

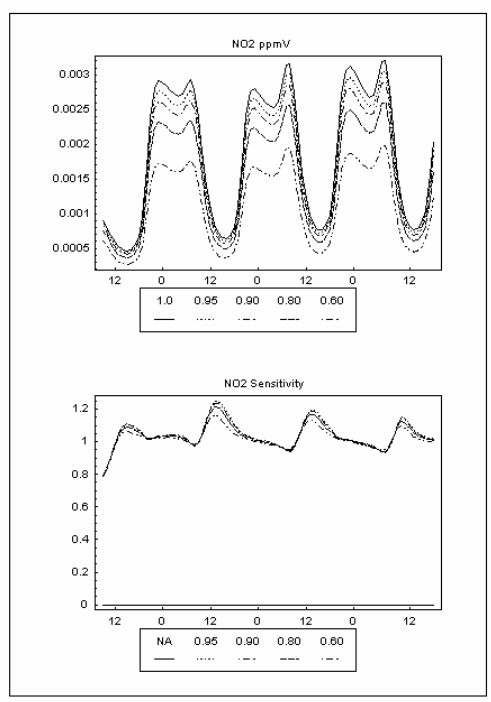

Fig. 2 Time series plot of mean NO2 concentration in the surface layer, and sensitivity of that mean to scaling of nitrogen emissions.

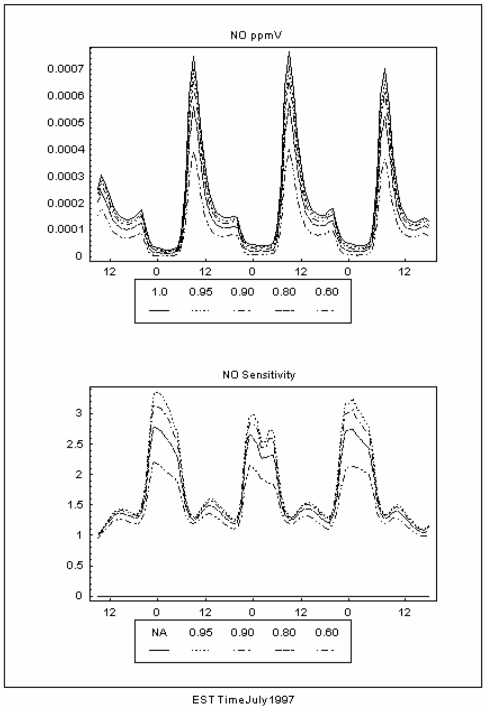

Fig. 3 Time series plot of mean NO concentration in the surface layer, and sensitivity of that mean to scaling of nitrogen emissions.

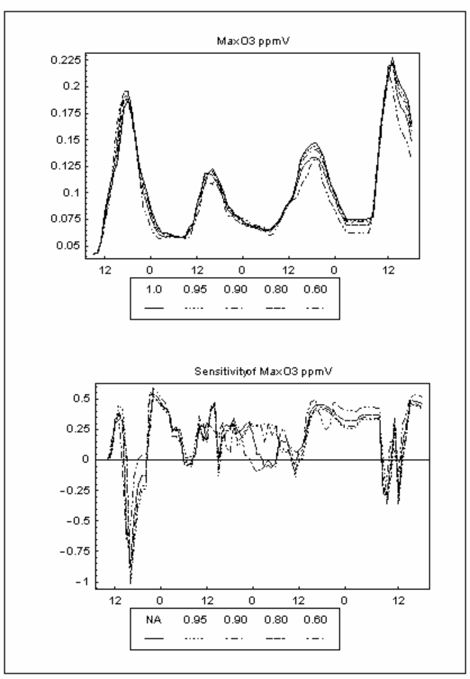

Fig. 4 Time series plot of maximum O3 concentration in the surface layer, and sensitivity of that maximum to scaling of nitrogen emissions.

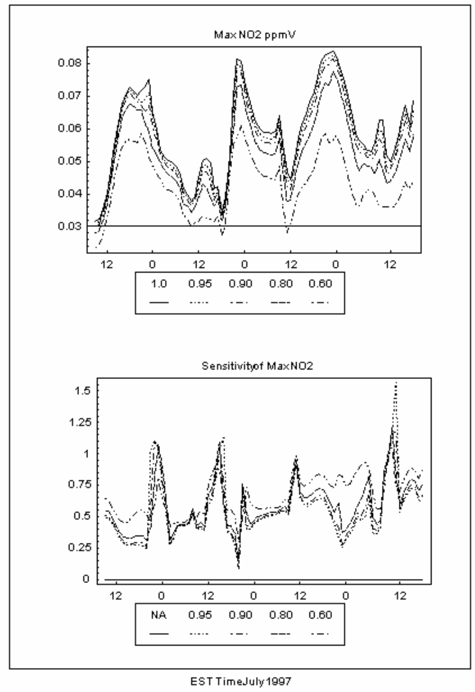

Fig. 5 Time series plot of maximum NO2 concentration in the surface layer, and sensitivity of that maximum to scaling of nitrogen emissions.

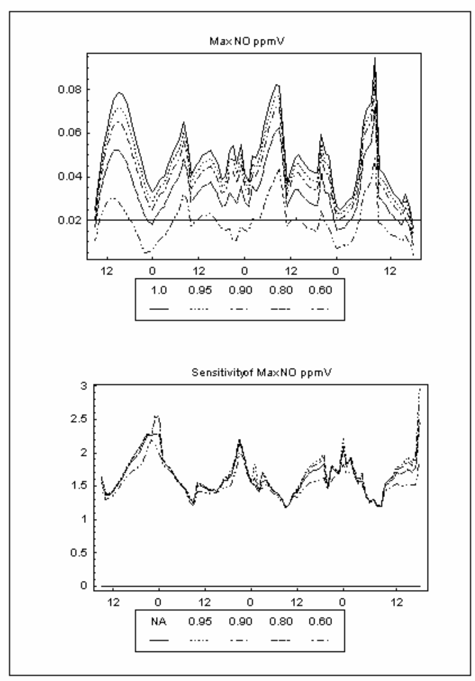

Fig. 6 Time series plot of maximum NO concentration in the surface layer, and sensitivity of that maximum to scaling of nitrogen emissions.