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An examination of the CMAQ simulations of the wet deposition of ammonium from a Bayesian perspective

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Abstract

The ability of the US Environmental Protection Agency's Community Multi-scale Air Quality (CMAQ) model to simulate the wet deposition of ammonium during 8-week winter and summer periods in 2001 is evaluated using observations from the National Acid Deposition Program (NADP) monitoring sites. The objective of this study is to ascertain the effects of precipitation simulations and emissions on CMAQ simulations of deposition. In both seasons, CMAQ tends to underpredict the deposition amounts. Based on the co-located measurements of ammonium wet deposition and precipitation at the NADP sites and on estimated precipitation amounts for each grid cell, Bayesian statistical methods are used to estimate ammonium wet deposition over all grid cells in the study region. To assess the effect of precipitation on the CMAQ simulations, our statistical method is run twice for each time period, using the simulated precipitation information provided to CMAQ and precipitation estimates based on data collected by the cooperative observer network. During the winter period when stratiform-type precipitation dominates, precipitation amounts do not seem to be a major factor in CMAQ's ability to simulate the wet deposition of ammonium. However, during the summer period when precipitation is mainly generated by convective processes, small portions of the region are identified in which problems with precipitation simulations may be adversely affecting CMAQ's estimates.
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Keywords: Ammonium wet deposition; Model evaluation; Bayesian statistical methods; Spatial correlation; Community multi-scale air quality (CMAQ) model; National acid deposition program (NADP); Ammonia emissions

1. Introduction

An important aspect in the development and maturation of an air-quality prediction model is the evaluation of the model's ability to predict fields of interest to the air-quality community. This paper focuses on the ability of the US Environmental Protection Agency's Community Multi-scale Air Quality (CMAQ) model to predict the wet deposition of ammonium. A complete description of the

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CMAQ model can be found in Byun and Schere (2006). Two critical elements in this analysis are the precipitation forecasts produced for CMAQ by MM5, a mesoscale meteorological model (Grell et al., 1994; Dudhia et al., 1998), and ammonia emissions. Our objective is to examine the effects of precipitation on the CMAQ simulation of the wet deposition of ammonium. Section 8.2 of Byun and Schere (2006) describes how CMAQ treats wet deposition. There is abundant observed precipitation data with which to judge the MM5 precipitation fields (see the data section). It should be noted that the current implementation of CMAQ does not include scavenging or wet deposition by snow or ice. This would contribute to model uncertainties during the winter season.

The wet deposition of ammonium is an important component of the total mass budget of ammonia/ammonium. Ammonium wet deposition has a detrimental impact on terrestrial and aquatic ecosystems. This is especially true for water quality. For instance, Sheeder et al. (2002) found that nitrate and ammonium were major factors in the decline of water quality in the Chesapeake Bay.

Ammonia emissions are an important factor in understanding and modeling the wet deposition of ammonium. A careful examination of the ammonia emissions data has been made by Gilliland et al. (2003) and Gilliland et al. (2005). Because the main sources of ammonia emissions are fertilizer application and animal husbandry, there is significant uncertainty in the seasonal distribution of the emissions. These two papers and those by Goebes et al. (2003) and Pinder et al. (2004) document the development of an improved ammonia emissions data set. These ammonia emissions data were used in our annual 2001 CMAQ simulation run. The following figures clearly show the problems that CMAQ has in simulating the wet deposition of ammonium. The observed data in these figures came from the NADP monitors. The CMAQ values were obtained at the NADP locations by kriging the CMAQ output fields.

Fig. 1 shows the relationship between the CMAQ simulation of the wet deposition of ammonium and the observed values. Clearly, CMAQ has underpredicted the deposition values in both seasons. The correlation coefficient is particularly low in the summer. We will examine some potential causes for this underprediction. Fig. 2 shows the relationship of the CMAQ deposition simulations to the MM5 precipitation simulations. As one would expect, the deposition values increase as the precipitation increases. The correlation coefficients indicate that the relationship is strong in the summer, but weak in the winter.

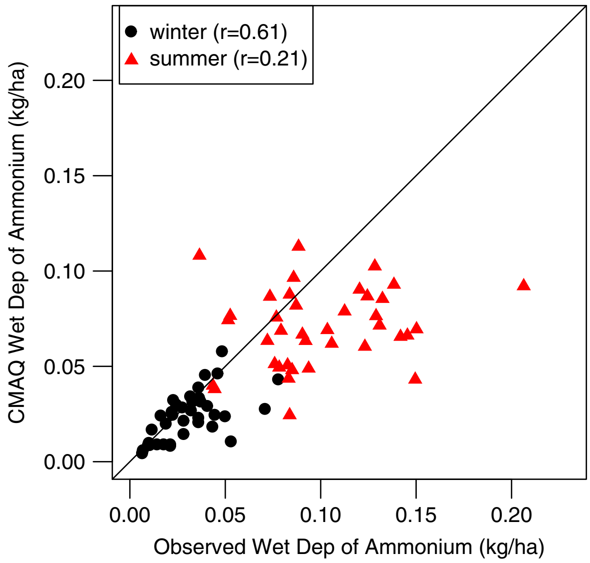

Fig. 1. CMAQ wet deposition of ammonium versus observed wet deposition of ammonium.

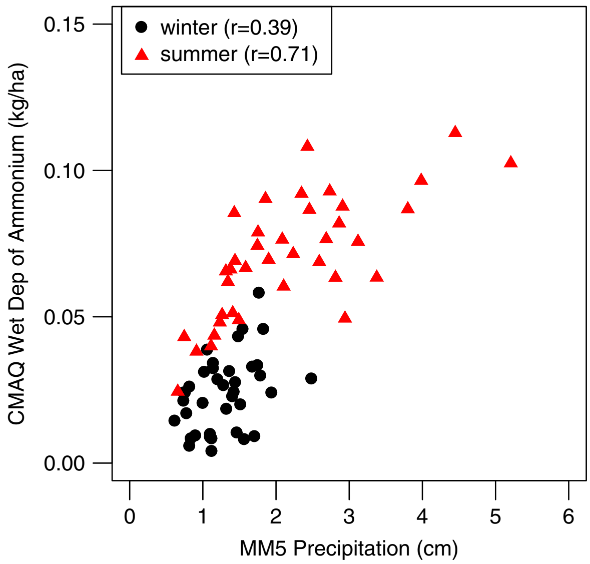

Fig. 2. CMAQ wet deposition of ammonium versus MM5-simulated precipitation.

Fig. 3 shows the relationship between MM5 precipitation simulations and the observed precipitation. The correlation coefficient for the winter is high, while for the summer it is somewhat lower. The convective nature of summer precipitation makes it harder for the model to predict, and this