

Comparison of organic nitrogen from CMAQ with measured values using a revised CB05 chemical mechanism

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Organic nitrogen is an important contributor to the total atmospheric nitrogen deposition. However, our understanding of the sources and composition of organic nitrogen is limited. In this study, we examine potential sources of uncertainty and error in the calculations of organic nitrate in air quality models. Treatment of organic nitrogen in regional air quality models is very limited due to gaps in the emissions inventory and the chemical mechanisms. Traditionally, chemical mechanisms developed for regional air quality models have focused on ozone chemistry and therefore organic nitrogen compounds such as urea are often speciated as VOCs rather than explicit nitrogen species. Additionally, organic nitrate compounds are lumped together to improve model runtime even though chemical properties may be quite variable. The chemical mechanism (CB05TUCL) was revised to include better consideration of the multifunctional character of organic nitrates, including increases in aqueous solubility and gas-phase reaction rates. These revisions also included recycling of organic nitrate and NO_x in the gas-phase reactions of organic nitrates. The assumptions made in these derivations are tested out in a series of sensitivity studies in which CMAQ predictions are compared to measurements of total organic nitrogen concentrations in precipitation at a site in Bondville, IL. The results of these studies provide insights on how to best represent a complex ensemble of chemical species in an air quality model and motivate further model and emissions inventory development.

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