Annual Model Simulations and Evaluations of Particulate Matter and Ozone over the Continental United States Using the Models-3/CMAQ System

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Brief Description:

EPA's Air Quality Modeling Group at Office of Air Quality Planning and Standards has been undertaking a series of model application and evaluation efforts over multiple (urban, regional, and continental) scales using the Models-3/Community Multi-scale Air Quality (CMAQ) modeling system developed by EPA. The objective is to establish the feasibility of using the Models-3/CMAQ system for applications on criteria pollutants such as PM 2.5 and ozone and related regional haze issues. As a pioneering effort, model simulations for the entire year of 1996 were conducted over the continental United States using a 36-km grid resolution. The first part of this paper is to examine the seasonal behaviors of Particulate Matter (PM) and ozone (O3) and their linkages, which were found to be closely linked to each other. A series of emissions sensitivity studies revealed that the responses of ozone and PM 2.5 constituents were highly correlated over the entire year. Over the summer months, NOx emissions reduction led to lower sulfate PM, mainly due to lower ozone and its related oxidants, while over the winter months, NOx reduction led to higher sulfate PM (but lower nitrate PM), mainly due to higher ozone as a result of less NO titration. The reduction of SO2 emissions, while leading to lower sulfate PM, appeared to allow the remaining available NH3 to react with HNO3 to form more nitrate PM.

The current modeling effort in this series of modeling studies is to conduct annual 2001 simulations over the continental US. This focus of this effort has been turned into the model evaluation by taking advantage of a much larger set of available ambient PM speciation data such as the Interagency Monitoring of Protected Visual Environments (IMPROVE), Clean Air Status and Trends Network (CASTNet), and the Speciation Trend Network (STN) network data in 2001. The preliminary results showed that the model simulated the sulfate PM very well over the summer months when sulfate PM was the dominant PM2.5 species. The model appeared to simulate the total nitrate (nitrate PM and nitric acid, HNO3) fairly well, but the partitioning between the nitrate PM and HNO3 lead to modest overestimate of nitrate PM. The model simulations indicated that the simulations of nitrate PM and HNO3 were highly sensitive to (1) amount of ammonia (NH3) emissions, (2) dry deposition of HNO3 and NH3, (3) nighttime chemistry of N2O5 and HNO3, and (4) diffusivity of nighttime mixing height. The model predicted no significant bias on the levels of organic PM, but the correlation coefficient was not very high, which revealed the scientific complexities in simulating secondary organic aerosols (SOA) formation and uncertainties in the primary SOA emission inventories.