Objective reduction of the model domain dimensionality for comparison of the performances of CMAQ and REMSAD models

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In the United States, developing emission reduction strategies aimed at achieving air quality standards is a responsibility of government agencies at the Federal and State level. To accomplish this mission, the agencies use photochemical air quality modeling systems because they allow testing of the impact of various hypothetical emission reduction strategies and facilitate decisions upon the most suitable alternatives. Among the prominent photochemical models available to accomplish this task are the Community Multiscale Air Quality model (CMAQ) and the Regional Modeling System for Aerosols and Deposition model (REMSAD). Because they are often used under different conditions (meteorology, emissions, etc), the relative performances of these models have rarely been extensively inter-compared. To facilitate comparisons, the U.S. Environmental Protection Agency (EPA) has recently simulated air quality over the contiguous United States during year 2001 with a horizontal cell size of 36 km × 36 km under identical conditions (same boundary/initial concentrations, biogenic and anthropogenic emissions, and meteorology). Our intention is to use these simulation results to determine the extent to which REMSAD and CMAQ can interchangeably be used to simulate PM2.5 and its constituents (more specifically, sulfate and nitrate).

Attempting to involve all pertinent data available in the evaluation process and clearly indicate whether or not CMAQ and REMSAD performances are similar is a challenge. Should evaluation metrics (such as gross errors (bias) or squared errors) be computed and reported individually for each day and observation site? Can days or sites be grouped without loss of valuable information? To address this challenge, we propose an evaluation procedure founded on the objective division of model domain into a limited number of zones corresponding to distinct modes or variation (i.e, zones where concentration changes happen concurrently) and assessment of models' adequacy within each of these zones. Rotated principal component analysis (RPCA) is the tool utilized to perform this spatial division of the domain. In an effort to differentiate the ability of CMAQ and REMSAD to reproduce short term (day to day) and long term (monthly) variations, the evaluation metrics (biases and squared errors) are calculated for each site and day when an air sample was collected, as well as for the monthly averaged observations and model estimates. These statistics are then averaged independently for each spatial group and month. By doing so, we are able to specify the regions and months best reproduced by each model. The statistical significance of the calculated differences between CMAQ and REMSAD evaluation metrics is tested. The proposed technique is illustrated with IMPROVE PM2.5, sulfate and nitrate measure-ments as the basis of comparison.

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