Performance of an Air Quality Model across a Range of Environmental Conditions

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Summary

Air quality impacts in the southern Appalachian Mountains of the eastern United States are under study by the Southern Appalachian Mountains Initiative (SAMI). SAMI is a non-profit entity made up of participants from various stakeholder groups. The goal of SAMI is to identify air pollutant emission reduction strategies that could be used to mitigate air quality-related impacts in sensitive ecosystems of the region.

Objectives – The objective of this paper is to summarize the performance of the air quality modeling done by SAMI across a wide range of environmental conditions. Understanding systematic variations in modeling error can lead to improved modeling applications in the future.

Modeling Approach – SAMI is investigating various emission reduction strategies using sophisticated environmental data bases and a suite of computer models. Air quality source-receptor linkages are being simulated using the Urban-to-Regional Multiscale (URM) Model. The URM model is a three-dimensional multiscale Eulerian photochemical model that accounts for the formation, transport and removal of pollutants in the atmosphere. URM has been enhanced to include aerosol dynamics through an equilibrium based aerosol module, wet deposition scavenging processes through the Reactive Scavenging Module, and heterogeneous chemistry. The modeling domain covered the eastern half of the United States. The nested model grid with the highest spatial resolution (grid cells of 12x12 km) was located along the southern Appalachian Mountain chain.

SAMI adopted an episodic modeling approach. Part of this approach was to develop a method for characterizing different time intervals (day or week) using a statistically-defined class. These classes, which varied by site and type of impact, were then used to select a set of multi-day episodes for detailed modeling. SAMI selected nine episodes to represent the full spectrum of ozone, deposition and visibility conditions. Results for a total of 69 days are available for analysis.

Ozone Performance – Ozone modeling performance was analyzed based on the maximum daily 8-hour average ozone mixing ratio, $[O_3]_{mx8}$, near the surface. Model error, e_i, for pollutant species *i* is

$$e_i = c_{mi} - c_{oi} \ ,$$

where c_{mi} is the model value and c_{oi} is the observed value. The modeling consistently produced $e_i>0$ when observed $[O_3]_{mx8}$ <60 ppb and produced $e_i<0$ when observed $[O_3]_{mx8}$ >60 ppb for all episodes. This behavior, seen before in other models, is believed to be caused by an inability of the modeling system (emissions, meteorological and chemical) to reproduce the full range of conditions that control ambient pollutant concentrations.

SAMI defined 4 ozone classes, with class 4 representing the most severe ozone events. Daily grid-averaged biases for ozone were sorted by SAMI pollutant class. Results presented here represent a composite view of model performance. The ozone class value was averaged for the two national parks (Great Smoky Mountains, TN and Shenandoah, VA) for which the classification scheme was devised. Hourly ozone bias was normalized by the actual observed ozone value. The normalized bias at noon on each modeled day that was classified and plotted. Most bias values fall within ±10% of zero for classes 1-3, but was usually biased low when the average ozone class was >3.

Aerosol Performance – Errors in computed aerosol concentrations were analyzed by species for particle sizes <2.5 μm ($PM_{2.5}$), and in terms of total mass for particles >2.5 μm ("coarse" PM). Bias patterns are similar to those for ozone, with underestimates for low levels and overestimates for high levels of particles. Model accuracy, based on the least-squares regression of model results versus observations, was found to be highest for sulfate and organic carbon, and poorest for nitrates, elemental carbon and crustal minerals. $PM_{2.5}$, with its strong dependence on sulfate and organic carbon, was simulated moderately well.

Wet Deposition Performance – Wet acid deposition model performance was evaluated by comparing simulated results to observations taken from the National Atmospheric Deposition Program (NADP) monitoring network. Species that were compared include sulfate, nitrate, ammonium, hydrogen ion, and crustal cations (Mg and Ca). NADP samples are collected once each week (Tuesday) so that concentrations and precipitation volume are only reported as 7-day cumulative values. There are 83 NADP monitoring sites in the modeling domain. However, only data from stations in the 12-km grid are used in this evaluation.

The large spatial variability in precipitation and difficulty modeling convective precipitation conspired to produce a poor match between model and observations. Therefore, NADP observations were compared to the *best* (i.e., closest in magnitude to the observation) model result within a 30 km radius of the monitoring site. Although the *cell* values sometimes have a tendency to miss the observed sulfate mass flux, the *best* values usually match well and were used in all the model performance calculations.

Sulfate and nitrate wet deposition are the species of greatest interest. Error in computed deposition is affected by error in both the aqueous concentrations of these species and the modeled precipitation amount. Modeled and observed anion levels, precipitation amount, and deposition fluxes were compared along with nitrate and sulfate molar concentrations for both modeled and observed data sets. Modeling overestimated precipitation considerably for light events and underestimated it slightly for heavy events. This bias pattern is reflected in the biases for sulfate and nitrate wet deposition. Modeling also frequently overestimated both anion concentrations in precipitation across the entire range of values. However, the influence of these biases does not appear to be as important as that of precipitation amount. It is interesting to note that the observed nitrate:sulfate molar ratio is near one for medium and high concentrations of the anions, but is much greater than one for greatly diluted levels. The latter are also often associated with light precipitation events. The model appears to do well in reproducing this ratio for the medium and high anion conditions, but URM never simulated conditions with high nitrate:sulfate ratios.

Conclusions – Model error for ozone, aerosols and wet deposition showed a consistent pattern with positive bias for low pollutant levels and precipitation amounts, and negative bias for high pollutant levels/precipitation amounts. This is probably caused by coarse spatial resolution, overly small emissions variance, overly smoothed turbulent mixing, and an inability to simulate sub-grid scale processes. Boundary conditions biased high may also have contributed to a high bias at low levels for $PM_{2.5}$.