Evaluation and Variability of Chemical Transport Models Sulfur and Nitrogen Compound Deposition and Ambient Concentration Estimates

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Sulfur and nitrogen deposition are critical variables for evaluating the potential for acidification of watersheds. Available deposition measurements have limited spatial coverage, lack high temporal frequency and have incomplete representation of all species. Thus, air quality models are increasingly used to develop estimates of dry and wet deposition of sulfate and nitrate compounds in watersheds in an effort to determine the acidifying deposition loads into the aquatic systems. However, these models need to be rigorously evaluated to ensure that one can rely on the modeled quantities instead of the measured quantities. In the U.S., these models are also being proposed to be used in establishing national standards based on modeled quantities. The U.S. Environmental Protection Agency (EPA) is considering acidification as the main ecological endpoint of concern in determining the secondary national ambient air quality standards for nitrogen oxides and sulfur oxides. Acidification is tied to depositions of sulfur and nitrogen, which are linked to ambient concentrations of the elements. As EPA proposes to use a chemical transport model in linking deposition to ambient concentration, it is important to investigate how the currently used chemical transport models perform in predicting depositions and ambient concentrations of relevant chemical species and quantify the variability in their estimates. In this study, three annual simulations by Community Multiscale Air Quality (CMAQ) modeling system and two annual simulations by Comprehensive Air Quality Model with Extensions (CAMx) for the entire continental U.S. domain are evaluated against available measurement data (including NADP) for depositions and ambient concentrations of sulfur oxides and reactive nitrogen species. The model performance results vary by evaluation time-scale and geographical region. Evaluation of annualized quantities (annual average ambient concentrations and annual total depositions) suppresses the large variances shown in the evaluation using the observation's native shorter-term time-scales (e.g., weekly). In addition, there is a large degree of bias and error (especially for deposition fluxes) in the modeling. The variability in the ratio of deposition to ambient concentration, so-called the transference ratio that EPA has proposed to use in linking deposition to ambient concentration, is also examined and are shown to vary considerably by geographical region and by model simulation.

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