High Time-Resolved Comparisons for In-depth Probing of CMAQ Fine-Particle and Gas Predictions

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ABSTRACT

Many atmospheric and chemical processes take place on time scales of minutes to hours. The processes at these time scales often critically determine the pollutant concentrations in the atmosphere. Most observations, other than ozone, are made at longer time scales, (e.g., daily or weekly) or are absent altogether. In this poster, two major sources of bias in the Community Multi-scale Air Quality Model (CMAQ) are examined with time-resolved data. One source is a physical process and the other is a chemical process. The physical source of bias stems from the meteorological inputs related to mixing, in particular the behavior of the simulated mixed layer in the evening. The chemical source of bias stems from the nighttime heterogeneous production of HNO_3 from N_2O_5. The analyses are carried out for summer and winter months to examine the seasonal dependence of the biases. The data are from the EPA Supersite Program and the Southeastern Aerosol Research and Characterization study (SEARCH) program for August 1999 (Atlanta), and July 2001 and January 2002 (Atlanta and Pittsburgh). First, the physically-based bias is examined. CMAQ's late afternoon rapid rise to over-prediction is very evident with inert tracer species such as elemental carbon (EC). The bias is greatest for urban areas and least for rural areas, though still evident. The bias is more significant in summer than winter for urban areas. The temperature bias in MM5 is consistent with the hypothesis that the bias is created by a premature collapse of the mixed layer in late afternoon. The physically-based bias creates situations of getting the right answer for the wrong reason (compensating errors) relative to 24-hour averages. This masks evaluation issues. An example for EC is shown in which 24-hour average comparisons look good, yet there is a significant mid-day under-prediction by CMAQ. This under-prediction is likely due to a missing emission source. Second, the chemically-based bias is examined using model sensitivity analyses. CMAQ includes the nighttime heterogeneous production of HNO_3 from N_2O_5 on wetted particles. CMAQ predictions with and without the nighttime heterogeneous were compared to measurements. Nighttime heterogeneous reactions have only a minor effect in summer, but have a major effect in winter where they are the most important factor affecting the overall winter HNO_3 budget. The daytime photochemical production of HNO_3 appears also to be too high.

Observations: (1) The performance of MM5 is important. The premature collapse of the

boundary layer which appears to be a feature in current predictions of MM5 can introduce important error in the diurnal variation of pollutant concentrations. The temperature bias also indicates other types of errors (e.g., in RH) that can affect aerosol processes. (2) Nighttime over-predictions can create compensating errors that mask model evaluation issues, making them invisible when only working with 24-hour averages (right answer, wrong reason). (3) Diurnal analyses allowed by high time-resolved measurements can uncover errors, such as errors in the emissions inventory. They can also uncover errors in the partitioning of semi-volatile aerosol species. (4) Diurnal analyses coupled with model sensitivity analyses can help probe for chemical process errors. Indeed, we found two issues with chemical processes when we were looking for one. (5) The two sources of bias explored here (one physical and one chemical) have roughly opposite seasonal dependencies. These findings could not have been identified without high resolution observations.

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