Modeling Atmospheric Particulate Matter:
Description and Evaluation of the CMAQ Aerosol Module (1.3)

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Atmospheric particulate matter (PM) is linked with acute and chronic health effects, visibility degradation, acid and nutrient deposition, and climate change. Accurate predictions of the PM mass concentration, composition, and size distribution are necessary for assessing the potential impacts of future air quality regulations and future climate on these health and environmental outcomes. The objective of this research is to improve predictions of PM mass concentrations and chemical composition, by advancing the scientific algorithms, computational efficiency, and numerical stability of the CMAQ aerosol module.

To achieve this objective, we have focused efforts on five areas in which previous versions of the CMAQ aerosol module were deficient. First, we doubled the computational efficiency of the aerosol module by improving the computations of coagulation coefficients and secondary organic aerosol (SOA) partitioning. Second, we worked with the developer of ISORROPIA, CMAQ's thermodynamic partitioning module for inorganic species, to smooth out discontinuities. Third, we developed a new parameterization of the heterogeneous hydrolysis of N_2O_5 as part of a larger effort to mitigate model overpredictions of wintertime nitrate aerosol concentrations. Fourth, we vastly improved the treatment of SOA by incorporating several new SOA precursors and formation pathways. Fifth, we implemented an efficient scheme to treat the dynamic interactions between inorganic gases and the coarse PM mode.

As a result of this research, the CMAQ aerosol module has been enhanced greatly over the past five years. During that time period, the aerosol module has been used for regulatory and forecasting applications (e.g., EPA-CAIR, NOAA-NCEP) because it is scientifically credible, computationally efficient, and numerically stable. With the recent scientific enhancements, our clients have increased confidence in the utility of CMAQ predictions of PM for future regulatory applications (e.g., RFS2 rulemaking). Meanwhile, the community of CMAQ users outside EPA continues to grow rapidly.