Atmospheric Chemistry Mechanisms: Current State and Future Needs (1.2)

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An accurate characterization of atmospheric chemistry is essential for developing reliable predictions of the response of air pollutants to emissions changes, to predict spatial and temporal concentrations, and to quantify pollutant deposition. In the past, air quality modelers have largely focused on single-pollutant issues, but it has since become clear that it is more appropriate to treat chemistry in an integrated, multiphase, multipollutant manner (National Research Council, 2004). For example, both inorganic and organic aqueous-phase chemistry can influence formation of secondary organic aerosol (SOA) through cloud processing (Carlton et al., 2006; 2007). High-NO_x versus low-NO_x conditions influence both ozone and SOA formation (Ng et al., 2007). In the past five years, our requirements for air quality modeling have also changed: the new National Ambient Air Quality Standards (NAAQS) for ozone and fine particulate matter ($PM_{2.5}$) have shifted our focus from urban-scale ozone episodes (~7 days) to regional/continental-scale simulations over longer time periods (one month to one year). In addition, our chemical mechanisms must adapt quickly to address emerging issues of high importance, such as changing climatic conditions and the impacts of biofuels.

The goal of our research in this area is to develop, refine, and implement chemical mechanisms for use in the Community Multiscale Air Quality (CMAQ) model to:

- Ensure that CMAQ and other models that are used for regulatory and research purposes have scientifically justifiable chemical representations, are appropriate for the application being studied, and are consistent with our most up-to-date knowledge of atmospheric chemistry;
- Ensure that interactions between gas-, aqueous- and particle-phase chemistries are adequately accounted for, so that we can truly predict multimedia chemical effects of emissions changes; and
- Develop techniques, tools, and strategies so that we are able to efficiently expand current mechanisms to predict the chemistry of additional atmospheric pollutants that we anticipate will become important in the future.

Our efforts to improve the chemical mechanisms in CMAQ have resulted in more complete and up-to-date descriptions of the important chemical pathways that influence concentrations of the criteria pollutants ozone and particulate matter. The inclusion of chlorine reactions and the explicit chemistry for 43 Hazardous Air Pollutants (HAPs) has helped to expand the applications for which CMAQ can be used. The inclusion of additional chemical detail in the aqueous and aerosol modules is providing pathways for more complete descriptions of secondary organic aerosol formation and decay.