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Modeling atmospheric ammonia and ammonium using a stochastic Lagrangian air quality model (STILT-Chem v0.7)

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Abstract. A new chemistry module that simulates atmospheric ammonia (NH_3) and ammonium (NH^+_4) was incorporated into a backward-in-time stochastic Lagrangian air quality model (STILT-Chem) that was originally developed to simulate the concentrations of a variety of gas-phase species at receptors. STILT-Chem simulates the transport of air parcels backward in time using ensembles of fictitious particles with stochastic motions, while accounting for emissions, deposition and chemical transformation forward in time along trajectories identified by the backward-in-time simulations. The incorporation of the new chemistry module allows the model to simulate not only gaseous species, but also multi-phase species involving NH_3 and NH^+_4. The model was applied to simulate concentrations of NH_3 and particulate NH^+_4 at six sites in the Canadian province of Ontario for a six-month period in 2006. The model-predicted concentrations of NH_3 and particulate NH^+_4 were compared with observations, which show broad agreement between simulated concentrations and observations. Since the model is based on back trajectories, the influence of each major process such as emission, deposition and chemical conversion on the concentration of a modeled species at a receptor can be determined for every upstream location at each time step. This makes it possible to quantitatively investigate the upstream processes affecting receptor concentrations. The modeled results suggest that the concentrations of NH_3 at those sites were significantly and frequently affected by Ohio, Iowa, Minnesota, Michigan, Wisconsin, southwestern Ontario and nearby areas. NH_3 is mainly contributed by emission sources whereas particulate NH^+_4 is mainly contributed by the gas-to-aerosol chemical conversion of NH_3. Dry deposition is the largest removal process for both NH_3 and particulate NH^+_4. This study revealed the contrast between agricultural versus forest sites. Not only were emissions of NH_3 higher, but removal mechanisms (especially chemical loss for NH_3 and dry deposition for NH^+_4) were less efficient for agricultural sites. This combination explains the significantly higher concentrations of NH_3 and particulate NH^+_4 observed at agricultural sites.

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