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Development of the adjoint of GEOS-Chem

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Abstract. We present the adjoint of the global chemical transport model GEOS-Chem, focusing on the chemical and thermodynamic relationships between sulfate - ammonium - nitrate aerosols and their gas-phase precursors. The adjoint model is constructed from a combination of manually and automatically derived discrete adjoint algorithms and numerical solutions to continuous adjoint equations. Explicit inclusion of the processes that govern secondary formation of inorganic aerosol is shown to afford efficient calculation of model sensitivities such as the dependence of sulfate and nitrate aerosol concentrations on emissions of SO_v, NO_v, and NH₃. The accuracy of the adjoint model is extensively verified by comparing adjoint to finite difference sensitivities, which are shown to agree within acceptable tolerances. We explore the robustness of these results, noting how discontinuities in the advection routine hinder, but do not entirely preclude, the use of such comparisons for validation of the adjoint model. The potential for inverse modeling using the adjoint of GEOS-Chem is assessed in a data assimilation framework using simulated observations, demonstrating the feasibility of exploiting gas- and aerosolphase measurements for optimizing emission inventories of aerosol precursors.

■ Final Revised Paper (PDF, 7837 KB) ■ Discussion Paper (ACPD)

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