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- Volumes and issues
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Development of the high-order decoupled direct method in three dimensions for particulate matter: enabling advanced sensitivity analysis in air quality models

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Abstract. The high-order decoupled direct method in three dimensions for particulate matter (HDDM-3D/PM) has been implemented in the Community Multiscale Air Quality (CMAQ) model to enable advanced sensitivity analysis. The major effort of this work is to develop high-order DDM sensitivity analysis of ISORROPIA, the inorganic aerosol module of CMAQ. A case-specific approach has been applied, and the sensitivities of activity coefficients and water content are explicitly computed. Stand-alone tests are performed for ISORROPIA by comparing the sensitivities (first- and second-order) computed by HDDM and the brute force (BF) approximations. Similar comparison has also been carried out for CMAQ sensitivities simulated using a week-long winter episode for a continental US domain. Second-order sensitivities of aerosol species (e.g., sulfate, nitrate, and ammonium) with respect to domain-wide SO_2, NO_x, and NH_3 emissions show agreement with BF results, yet exhibit less noise in locations where BF results are demonstrably inaccurate. Second-order sensitivity analysis elucidates poorly understood nonlinear responses of secondary inorganic aerosols to their precursors and competing species. Adding second-order sensitivity terms to the Taylor series projection of the nitrate concentrations with a 50% reduction in domain-wide NO_x or SO_2 emissions rates improves the prediction with statistical significance.

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