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Geoscientific
Model Development
Discussions

Interactive comment on "Development of the high-order decoupled direct method in three dimensions for particulate matter: enabling advanced sensitivity analysis in air quality models" *by* W. Zhang et al.

Anonymous Referee #1

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This paper presents and evaluates the extension of the decoupled direct method to compute higher-order sensitivities for particulate matter in the CMAQ model. Implementation of high-order DDM sensitivities for PM had not previously been accomplished in a photochemical model and is a substantial undertaking given the complexities of the ISORROPIA inorganic aerosol module. This work thus provides a significant contribution to the toolbox of approaches for modeling responsiveness of air pollutants to emission controls and other perturbations. This journal is an appropriate forum for presenting such work, and the paper should be published upon addressing the fol-

lowing comments. MAJOR COMMENTS: 1. All of the discussion and results relate to sensitivities to emissions. Please clarify whether CMAQ-HDDM-PM has been implemented and validated for other types of parameters (reaction rate constants, initial conditions, boundary conditions, etc.) as well. Also, are there opportunities to extend HDDM-PM to consider sensitivities to parameters in ISORROPIA such as equilibrium coefficients? I expect that this would be beyond the scope of the current work, but the authors could comment on the feasibility of this, as it may be useful for uncertainty analysis studies. 2. It would be informative to present performance statistics for the HDDM vs BF comparisons, either in the figures or as supplementary tables. This would provide useful benchmarks for others who may seek to implement HDDM-PM in other models, or to see how performance improves as the cloud DDM issues get rectified. 3. Insufficient testing is presented to evaluate the performance of Taylor series expansions, which are likely to be the primary application of this work. Only the relatively easy case of nitrate vs ENOx is shown in Figure 8. Performance should also be checked for at least one more challenging case such as nitrate vs ESO2, and evaluated at a few different levels (including -100% for ZOC) rather than just -50% to test the range over which local sensitivity coefficients can be extrapolated reliably. In these tests, performance should be compared for Taylor series expansions driven by BF and HDDM coefficients; this should be straightforward to do, since all of the necessary sensitivities have already been computed, and would provide a useful gauge of the relative utility of BF and HDDM sensitivities. SPECIFIC COMMENTS: p. 2607, line 17: The equations don't show subscripts for location. p. 2609, line 19: The wording implies that Ri represents only reactions of i, but presumably chemical production of i from other species is also accounted for in dC/dt. p. 2611: The S's in Eqs 4-5 and 6-7 have different meanings and units, so it may be clearer to denote them differently. p. 2612, Eq 10: Why does this equation differ from K4 in Table 1? p. 2613, line 17: This point is repeated on p. 2619, so could be deleted here; or, at least remove the word "always". p. 2614, line 2: The log in the subscript is inconsistent with how these are written in Eqs 11 and 12. Please clarify which is intended. p. 2614, Eqs 14-15: Sensitivities to

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what. For example, do you mean S(1)H2O,p1? p. 2617, lines 10-11: It is unclear what is meant by this statement. Do you mean that HDDM agrees better with BF computed by +/-50% changes than by +/-10% changes? That would be surprising, since bigger perturbations would have more opportunity to shift to a different subregime of ISORROPIA that wouldn't be represented by the local HDDM coefficients. p. 2618, lines 15-16: It's not that BF is inaccurate for describing nonlinear response, since a series of BF simulations could characterize PM concentrations for various emissions levels as is done in response surface modeling. The point is that this particular approach of extrapolating from BF coefficients derived from Eqs 1 and 2 may not reliable. TYPOS: p. 2612, line 8: coefficients p. 2615, line 12: Change incremental to increment p. 2615, line 21: The + on NH4 should be a superscript p. 2616, line 4: Change are to is p. 2616: Correct the spelling of Grell and Roselle Figure 7 caption: calculated Figure 8 caption: series

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Interactive comment on Geosci. Model Dev. Discuss., 4, 2605, 2011.

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