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Atmospheric Chemistry and Physics Discussions

Interactive comment on "Development of the adjoint of GEOS-Chem" *by* D. K. Henze and J. H. Seinfeld

Anonymous Referee #3

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Comments on "Development of the adjoint of GEOS-chem" by Henze and Seinfeld.

This paper reports on an impressive piece of work - a development of an adjoint for the GEOS-chem model including aerosols and chemistry. The accuracy of the adjoint is tested by evaluating the adjoint sensitivity against the sensitivity of the forward model in a number of idealized tests. With the exception of the advection scheme the tests confirm the accuracy of the adjoint solution. The paper concludes by discussing some of the sensitivity analysis and inverse modeling test results. The paper is mostly well written and clear. The care with which the authors check their solutions is also commendable.

That said, publication of this work seems somewhat premature. However, I encourage the authors on this very exciting endeavor. The scientific payoffs should be large.

1) The authors have apparently not found a suitable adjoint for the advection scheme. While they claim this is not the focus of their work, advection is such a fundamental process that it casts doubt on the adjoint model as a whole. The adjoint may give suitable answers when global sensitivities as a whole are evaluated over short time periods (less than a day). However, there appear to be some real problems with it. a) Evaluating the cost function regionally leads to large discrepancies. This seems to severely limit the type of data which can be used: it precludes using regional data and it necessitates long data assimilation windows when using satellite data. As the adjoint solution deteriorates over long integration times it is not clear under what circumstances one can use this adjoint in realistic data assimilation problems. b) The authors claim that this could be an impediment if only sparse or infrequent measurements are available. There is a large gap between "sparse and infrequent measurements" and global sensitivities. At what spatial and temporal scales will measurements be of value? c) The solution deteriorates dramatically with long assimilation windows (even 2 days). Yet most satellites do not achieve global coverage in even 2 days. What global measurement system do they envisage using with rapid global coverage? d) The authors state that this deterioration of the adjoint will be more critical for longer lived species whose distributions are chiefly determined by transport. Certainly this applies to aerosols which are transported over thousands of kilometers. What type of species do they expect to be able to use in realistic analysis? e) The discrepancy seems to get worse at high sensitivities. Aren't these exactly the points which yield the most information about the solution? While I can understand the authors' reluctance to further explore the adjoint of the advection scheme, and while I realize the advection scheme is not the authors' primary interest, transport is intrinsic to the problems they are addressing. Did they authors consider implementing another advective scheme more amendable to adjoint solutions? The authors have failed to show that their system is adequate for realistic data assimilation and inverse problems. Slope biases of 0.8 to 1.3 seem very significant for such an idealized test. Furthermore, the points listed above need

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to be adequately addressed. I think it is incumbent on the authors' to show they have produced an adjoint which is adequate for use under realistic conditions.

2) This paper seems to be an application paper instead of a numerical methods paper I believe many of the numerical methods used have been published elsewhere. While I commend the authors for their careful checking of the adjoint solution, and while the tests they conducted are necessary checks on their modeling system, these checks should not be the focal point of the paper. It would be sufficient to state that tests are conducted and the adjoint solution is accurate to x% (with perhaps one figure) and then to go on and apply the system to a real scientific problem. In other words the checks on the adjoint, which are certainly necessary, do not make a paper. (I suspect one reason separate checks were performed on different modeling components is to identify the advective adjoint as a problem. This would not have been necessary if a more accurate adjoint of the advective scheme had been found.). The "science" in the paper seems rather haphazard - more in the vein of showing the power of the adjoint, instead of investigating a scientific problem in depth. The paper needs to be science driven.

3) I am puzzled by Equation (14). Why is it necessary to find the adjoint variable with respect to the parameters iteratively (page 10599). Usually this variable can be found through a direct application of the adjoint.

4) The units on page 10604 are puzzling. The units given for emissions are valid for a source (i.e., emissions should molecules/(cmˆ2 s), not molecules/(cmˆ3 s)). Then the adjoint sensitivities of concentrations with respect to emissions should then be in units of sec/cm.

5) The authors' state on page 10611 that the "diffusive nature of [first order, upstream, linear transport schemes] actually increases the bias". This is not at all clear to me. In fact linear (and hence diffusive) advection schemes are known to give accurate adjoints. Can the authors justify this statement?

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6) I am also puzzled by the derivation of the continuous adjoint (pages, 10607, 10608). One should not get equation (26) (an equation in flux form) from the advective form of the tracer continuity equation (equation 25) without additional assumptions.

7) To be of value inverse problems need to involve many degrees of freedom as one attempts to localize the emissions. If I am not mistaken Figure 9 involves solving for a multiplicative factor for global emissions, and thus only involves a few degrees of freedom. While this “toy” problem is certainly important as a first test for checking ones solution, it is not sufficient to provide a rigorous test of the adjoint solution.

Interactive comment on Atmos. Chem. Phys. Discuss., 6, 10591, 2006.

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