

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

Anonymous Referee #1

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General comments This paper provides details on the development and validation of GEOS-Chem adjoint model. This will facilitate the further development of chemical data assimilation using the GEOS-Chem model. In addition, such documentation helps the similar projects involving other chemical transport models. The paper is very well written and clearly presented. It is recommended for publication after minor changes.

Specific comments

1. line 100 after Equation (1), “... species observations mapped to the model domain space ...”: The more common approach would be mapping variables from model space to observation space. It is sometimes impossible to do it the other way. Please comment on this.

2. line 197, “We use $\delta\sigma=0.1-0.01 \dots$ ”: The value of “ $\delta\sigma=0.1-0.01$ ” used to calculate the derivatives seems too big. Please explain why such a range is chosen. In addition, the derivatives calculated using $\sigma=0.1$ would be significantly shifted from the adjoint counterpart. That is, the derivative by the one-sided finite difference is indeed at $\sigma + 0.05$ while the adjoint gives the derivative at σ .
3. line 212, “... though these methods are used mostly in other fields”: Does this imply that the methods cannot be applied here?
4. line 243, “hence, λ has units of s^{-1} ”: Please differentiate adjoint state variables and the adjoint derivatives. The units appear to be s rather than s^{-1} .
5. line 258 and Table 1: Please provide references for full names of the species.
6. line 263, “the ratio $\lambda_{ENOX}/\Lambda_{ENOX}$ becomes 1.07 and 0.94”: Those numbers are not close enough to 1. It might be due to the way the finite difference was carried out, as mentioned previously. If it cannot be improved, please elaborate possible causes.
7. lines 583-585, “... however, this would risk over-optimization ...”: What is *over-optimization*? The possible oscillatory behavior is not due to more iterations. It could indicate that the problem does not have a unique solution. Please clarify.
8. lines 661-662: Please define RTOL and ATOL.
9. Figures 1-2: It is better to present the distribution of $\lambda_{ENOX}/\Lambda_{ENOX}$ in place of λ_{ENOX} or Λ_{ENOX} for the purpose of validation.
10. Figure 4: Consider using log scales for some of the plots.

Technical corrections

1. line 11, "... have a nearly 1:1 correlation and ...": It is not accurate to state "1:1 correlation" as the ratio is independent of the correlation.
2. line 187: "is know" => is known.

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

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