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Atmospheric Chemistry and Physics Discussions

Interactive comment on "Singular vector decomposition for sensitivity analyses of tropospheric chemical scenarios" *by* N. Goris and H. Elbern

Anonymous Referee #3

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This work presents application of singular vector analysis to photochemical box model simulations. This is an important step towards performing targeted observations for chemical systems. While that may not be the most relevant application given the extent of the results shown here, there has been only one other study of singular vectors in CTMs prior to this work. Thus it is a significant step forward in model diagnostic tools. Overall, I think the authors can clarify the connection of their results as stand-alone insights, and together with my comments and those of other reviewers arrive at a more focused manuscript which will be a valuable publication in ACP.

1 General comments

- This work would benefit from including more discussion of the merits of singular vector analysis vs other modes of sensitivity calculations (brute force, DDM or adjoint) for sensitivity studies of box-model photochemical calculations. How would they differ in their overall effort? What are the differences in the results they would provide? How well do the different methods scale when considering application to 3D CTMs?
- There seems to be a disconnect between the reasoning for this study described in the introduction (targeted observations) and the actual application (sensitivity of a photochemical box model). Discussing how singular vector analysis will eventually be useful for targeted observations is motivational, but perhaps not the most direct application of the results that are actually presented here. Could the authors instead find other applications of the kind of results they are generating in this initial application? For example, that NO_x emissions have impacts according to the time of their emission is relevant to discussion of pollution control strategies. The temporal trends in the singular vector growth has implications for inverse modeling of emissions and the degree to which observations may reflect uncertainties in concentrations several days prior or several hundred km afar. I would encourage the authors to find more direct ways of making their existing results relevant.
- Clearly this approach generates more results than can be discussed in the paper. In some cases, the authors choose to focus on results from particular scenarios. Could they explain a bit more why they pick specific scenarios to plot the results over others, such as MARINE for Figs 4 and 5? At the moment it seems a bit arbitrary at times.
- Regarding the box model, from what I can tell it contains only emissions and re-

actions. There are no loss rates or dilution factors. Wouldn't this lead to buildup of chemical concentrations beyond typical values? Is this perhaps why the influence of some perturbations is so pervasive across multiple days, while in the real atmosphere it is typically assumed that the influence of NO_x emissions are much more localized?

2 Specific comments

- The abstract could contain less general background material, and more about the results of this paper.
- 16754: Is the definition of the different families a bit arbitrary? Could one instead use the singular vectors themselves to define appropriate groupings?
- 16761: In equation 46, why not use the previous definitions of FWD and TLM model (i.e., M and L)?
- 16761: In eq 47, doesn't this not rule out the possibility of cancelation of errors by checking the dot product on the left and right sides rather than the individual components? I realize it's much more computationally efficient to validate using this metric, but for box-model simulations I would think that element-by-element checking would not be overly burdensome.
- The ability to follow discussion related to individual chemical components would be greatly enhanced by providing a definition of the species abbreviations.
- Section 4.1: Does the second conclusion (on pages 16768/16769) apply to all scenarios, even FREE and URBAN?
- I found it a bit odd that there wasn't much or any discussion of the NO_x results in section 4.3.1 and 4.3.2.

- 16746.18: no comma after reveal
- Overall, the grammar and punctuation is far from perfect and somewhat distracting. Below are listed a few places where it actually clouds the understanding; the entire paper would benefit from a thorough editing.
  - 16748.25: Point 1
  - 16768.23: that the results resemble
  - throughout, "to which extent" should be "to what extent"
  - 16779.27: "is at disposition"

Interactive comment on Atmos. Chem. Phys. Discuss., 11, 16745, 2011.