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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 #1

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The authors apply the method of singular vector decomposition, in order to perform a sensitivity analysis for a box model representing tropospheric chemistry. They concentrate on ozone formation.

As I was not a reviewer during the pre-ACPD phase of this manuscript, this is my first chance to comment on it.

General comments:

The singular vector decompostion is applied for the determination of the sensitivity of _one_ single variable (ozone concentration at the end of the box-model run) with respect to a few input parameters (initial concentrations or emission factors of chemical

species). For this task the application of an adjoint model or, in the case of only a few parameters of interest, even "brute-force" runs of the original model (modifying one parameter per run) would be sufficient - and even superior to the singular vector decompostion (SVD), which has the following disadvantages:

1) The programming effort before running the SVD is large.

2) The numerical effort (CPU time) of the SVD is very large.

3) Singular vectors, as presented in the manuscript, are normed (norm = 1). That is why they can represent only _relative_ sensitivity measures (importance of one species _relative_ to another one).

4) As both the vectors v and -v are singular vectors, the information on the sign of sensitivity is lost. However, this is an important information: for instance, as correctly pointed out by the authors, an increase of the initial NOx concentration may lead to an increase or decrease of the final ozone concentration, depending on the conditions (initial values) considered.

The authors seem to be aware of this general problem, because in the abstract, introduction, and summary they stress the usefulness of the singular vector decomposition for solving another problem: optimization of measurement configurations of chemical compounds. However, contrary to the statement at the beginning of the summary, this topic is not even mentioned in the main body of the manuscript. Now the main logic behind the manuscript appears to be: "In order to demonstrate that method M1 (singular vector decomposition) is suitable for problem P1 (optimization of measurements), we show that it works for a related problem P2 (sensitivity analysis), which can be solved better by a simpler method M2 ('brute-force' sensitivity analysis or adjoint model)".

Specific comments:

The results are very detailed, probably too detailed for the majority of the readers. The individual analysis of the impact of several (groups of) chemical species (NOx, VOC,

CSL, XYL, TOL, MGLY etc.) for 8 categories of model runs (different initial time and length of the simulation) for 6 different scenarios (LAND, MARINE etc.) makes it difficult to present a "take-home message" for the reader.

Technical comments:

Most parts of the manuscript are technically well written, containing some minor errors, e.g.:

- page 16748, line 12: "linear combination of 9 initial species'" should be "9 linear combinations of initial species'" (cf. Khattatov et al., 1999, p.18724)

- reference "Sandu et al. (2006)" should be "Liao et al. (2006)"

- Equ. (38) is a system of ordinary, not partial, differential equations.

- Fig. 4 is probably wrong (now it is a copy of Fig. 5)

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