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Interactive comment on "Sensitivity analysis by the adjoint chemistry transport model DRAIS for an episode in the Berlin ozone (BERLIOZ) experiment" *by* K. Nester and H.-J. Panitz

Anonymous Referee #1

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Review of paper: "Sensitivity analysis by the adjoint chemistry transport model DRAIS for an episode in the Berlin ozone (BERLIOZ) experiment" by: K.nester and H.-J. Panitz

This paper presents an analysis of a specific polluted event over the region of Berlin in Germany. This event was well documented by the way of the BERLIOZ experiment during the summer of 1998. The originality of the paper is to use a dedicated adjoint model to estimate sensitivities of ozone concentrations to model parameters. The sensitivity results are used to define a simplified data assimilation framework.

However, some important lacks were found in the paper. Even if the model develop-

ments are impressive, its use is not always as it is necessary. This leads to a large number of questions about the conclusions as presented by the authors. We present in the following the most important questions thinking that answers would improve the quality of the paper.

The adjoint approach is a powerful tool to estimate alltogether sensitivities to one pollutant. But, a realistic determination of a cause can only be perform if some hypothesis are carefully considered:

1. the model is perfect i.e the parameterizations used during the calculations can not be at the origin of an erroneous calculated sensitivity.

2. all parameters are taken into account: to "forgot" one model parameter biases the answer of the system and can put some high sensitivities values on a parameter for bad reasons.

About 1., in the text, the parameterizations used in the model are poorly described: for example, an important part of the discussion is devoted to the reactions rates. Even if the mechanism RADM2 is well known, there is no introduction of the mechanism: in section 2.1, the authors could give, at least, the number of reactions and model species, for example. This discussion may be important for this study: how reacts the RADM2 under various chemical regimes, NOx or VOCs limited? Is this point be an element to explain the underestimation in the plume, only far from the city and not near the city? (i.e a change in the chemical regime). On the other hand, the appendix A has no interest. We don't want to know the symbol used in the model or the species number. But we need to know the degree of confidence which one can put in the simplified chemistry represented in this mechanism (compared to another mechanism for example).

About 2., in the section 1, the authors postulate the parameters to be studied are initial and boundary conditions, emissions and reactions rates. Why not meteorological parameters? Is the used meteorology supposed to be perfect? or enough realistic

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for this study? Please justify this very important hypothesis. To assess this point, some comparisons between measurements and model are required. For example, a boundary layer height accurately estimated over the city but not in the plume may explain the ozone underestimation of 15%.

The vertical atmospheric column is splitted into four separate parts: why these fixed altitude? Do the authors considered that the layer 4 with a thickness of 75m (why 75m?) represents a realistic surface layer thickness for the whole period and over the whole domain?

The assumption in the section 3.1.2 is not clear. Why the deposition velocity was "slightly" modified? How much is slightly? For all other known chemistry-transport models, this specific assumption is not existing. What the impact of this hypotheiss on results?

In the section 3.1.4: "because good agreement may be obtained for some sentivities although there is still an error in the code". I'm very surprised of this sentence. Numerous tests exist to check the exact accuracy of every adjoint code. The authors have to check the accuracy of their adjoint model, using the Taylor test for example.

In the section 3.2: All the calculations are not clear. Why replacing P by P0xfacP? The authors have to give more explanations about the interest of a parameter change for the results as well as to justify for the choice of P0 and, finally, explain what is exactly facP.

In the section 3.2.1, the species names as acronyms are not useful. Some sentences "CO is still found between HC8 and OLI" are difficult to understand, not enough accurate. This section is only descriptive. Please explain what can be learned from these results.

In the Table 2, the sensitivities to photochemical equilibrium and NO emission were previously discussed in others papers. This is why it is bettre to use Ox. The fast

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titration of ozone by NO, for example, is a well known process leading to high sensitivity but only over short time periods and only over the sources. Thus, this can not explain the discrepancies found far from the city in the plume. Another obvious point is the sensitivity of ozone to its own boundary conditions. For the rest, of the Table, to refer only to the numbers of the reaction is not an easy way to see the results. To report directly and entirely the reactions would be certainly a better way for the reader.

Figure 2: What is the meaning of "ozone concentration distribution" How is used "distribution" in this context? Is it "surface ozone concentrations fields"?

p.6: replace "chapter 4" by section 4.

section 2.3 "averaging the simulated ozone ..." what corresponding periods? the text is not clear on how are estimated these values.

Finally, the adjoint method is well known to be efficient only for infinitesimal perturbation. Can the author explain why they chose this method whereas they want to explain an important discrepancy, between model and measurements. According to me, 15% on ozone concentrations can not be seen like "infinitesimal" error.

Interactive comment on Atmos. Chem. Phys. Discuss., 5, 8715, 2005.