**Atmospheric
Chemistry
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Discussions**

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 #2

Received and published: 12 October 2005

The paper by Nester and Panitz describes the application of the adjoint of a regional-scale chemistry transport model to identify possible reasons for the underestimation of ozone mixing ratios downwind of the city of Berlin for one particular day. It is well known that air pollution models, both on the global and local scale, still have deficiencies and do in some cases fail to reproduce observations. The search for reasons of these deficiencies is an ongoing task. Adjoint models are a particular useful tool to compute sensitivities of model results with respect to input parameters and may therefore give hints on possible reasons for differences between models and observations. I think the subject of this study is well adapted to ACP, and the study itself is suffi-

ciently original (with respect to the particular model and episode the adjoint model is applied to) for publication. However, I have serious concerns mainly about the design of the experiments (or the missing justification of this design), the presentation and (also often missing) interpretation of the results, and the in some places careless use of mathematics and language. Therefore I would recommend publication of this paper after careful revision. My main questions and points of concern are listed below in the order of appearance in the text.

Abstract
"... the most effective method of calculating the sensitivities is the application of the adjoint model." This sentence is appearing, in a very similar formulation, three times in the text. First it should be made clear how the effectiveness is defined. It should not be forgotten that the development of an adjoint model is time consuming. And even if effectiveness is defined with respect to computer time this sentence is not true as a general statement. Adjoint models are only useful for computing the specific type of "backward sensitivities" like in this study. "Forward" sensitivities (answering the question which model result is influenced by a specific parameter) can be well treated with forward or tangent-linear models.

1 Introduction
I agree, that it is not necessary to repeat in each paper all earlier efforts in the respective field of work. However, lots of things are completely missing in the introduction: The applied method (adjoint modeling) should be briefly discussed with its advantages, problems, and the history in the application in similar studies. Also, the authors should try to set the context of this study. Is the problem of underestimation of ozone in city plumes a general one or a specific problem of the KAMM/DRAIS model. Can people draw general conclusions from this study or is it useful only to identify error sources in one particular model. And which parameters have been identified in earlier studies (not necessarily adjoint model applications) as those ozone may be sensitive to.

2.3

Last sentence: "This result indicates that the ozone concentration ...". First, I doubt the usefulness of the choice of the three regions (Fig. 7) when the main aim is to explain differences at the Menz station. Given that the station is very close to the border of regions 2 and 3, and a wind speed of about 5 m/s, the air masses are feeling the production rate in region 3 maybe only for half an hour. Second: I agree that the comparison of production rates computed from observations and the model suggests that this is a probable reason for the described discrepancy between model and observations. However, the authors do not link this to their choice of parameters for the sensitivity study. Of course, all considered parameters do influence the chemical production more or less directly. But there are other parameters which should also be discussed, like deposition velocities and the mixing layer height. In particular this last parameter should be mentioned. Earlier, the authors mention that meteorological parameters are simulated well, but mention only the winds. Is this true also for temperature, cloud cover and the boundary layer height?

3 Sensitivity analysis
Definition of the distance function: The math notation used in the paper is very uncommon and renders the reading difficult. Why do the authors use combinations of letters (DF, FacE, Sif etc.) for variables? Symbols with sub- or superscripts as generally used for mathematics would be much easier to read. The cost function, e.g., is called J in the large majority of studies where such a function is used. Ide et al. (JMSJ, 1997) have suggested a unified notation for data assimilation. I would suggest that authors who are publishing in this area should try to follow these suggestions whenever possible.

3.1
The "definition" of adjoint operators and variables mixes general elements with others specific to this application. Adjoint operators and variables are not defined by equation (2). If the authors don't want to give a sound mathematical background of adjoint modeling they should give a reference and explain the basic principles of an adjoint model. For readers who are not familiar with adjoint models it is very difficult from the

definition given here to understand what an adjoint model does, and what an adjoint variable is (also a derivative). I find also the subsequent description of how the model is coded difficult to understand. The authors might first explain what different options exist and then say which option they (and maybe others) have chosen. The statement that "the adjoint DRAIS is coded in a similar way as the original and tangent linear models" does no help the reader who doesn't know about the coding of these models.

3.2
Definition of the sensitivity: Adjoint models compute gradients and not quotients of finite differences.

The reason for introducing FacP should be explained.

3.2.1
Do I understand correctly that all sensitivities presented are local maxima in the sense of S=max(Si) with i=1,N and N being the number of model grid boxes? Or only boxes of the surface layer? Or the maximum over all time steps? If not the latter, are they integrated over the time of simulation? And what is this time? There may be reasons for presenting local maximum values. However, these reasons should be explained. Another option would be to present an integrated sensitivity over the whole model domain. Such results could be presented additionally in the figures 9 to 14 and in the tables. For different variables, local maxima may occur at very different locations on the model grid. E.g. the influence of NO emissions is probably very different in grid boxes adjacent to the observing sites and further upwind, probably even of different sign. At least in the case of reaction rates where one could assume that a possible error would be similar in the complete model domain I don't see the sense of presenting local maxima. These issues have to be discussed, in particular with respect to the goal of this paper.

In the case of hydrocarbon emission it may be a good idea to present an integrated sensitivity to all species. Then the comparison to NOx would make more sense.

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3.2.2

The sensitivity to initial values is approaching zero the further backward in time the simulation is started. The sensitivity to emissions and boundary conditions, on the other hand, would approach a maximum value. Therefore, it makes no sense to compare sensitivities to emissions, boundary conditions, and initial values without giving the time of initialization. And this time should be defined and discussed with respect to the goal of the study. Independently of the time chosen, it would be interesting to present additionally results for a an integration time sufficiently long to reach steady values.

3.2.3

"This is the same ... but the sign is different." Here and in the other places the authors should give physical explanations for their results.

3.2.4

I would assume that errors in photolysis rates are not completely independent but all depend on the correct representation of absorption and scattering in the atmosphere. E.g., an incorrect representation of cloud cover would influence most photorates in a similar manner. That's why I would like to see a comparison of the integrated sensitivity to all photorates in comparison to the single ones.

4 Variation of relevant parameters

What is the reason for doing this? What is the additional information that can be gained after having done the sensitivity studies? I would also like to sea a discussion on the consequences of using a simplified assimilation approach. It is stated that "there is no intention to carry out a full data assimilation". Why not? Again, these issues should be discussed with respect to the goal of this paper.

How are emissions modified? I assume that they are time dependent in the model.

5 Conclusion

The authors clearly state their goal: "A sensitivity study was carried out to find the

reason for this underestimation" [of ozone]. However, they are less clear in saying if they have reached this goal. The reader is left with a ranking of sensitivities, five very different parameters to which ozone is similarly sensitive. The authors should discuss the probability for these parameters being the reason they were looking for, or if their change would only compensate other errors. I admit, this is not always easy. However it seems possible for several parameters: Photolysis rates can be measured. Probably they have been measured also in the BERLIOZ experiment. If reaction rates are systematically wrong, one should observe an improvement in the simulations for other simulated days, and observation sites. The same is true for emissions. If NOx emissions are systematically overestimated, the same reduction at other days should also provide an improvement in the simulations. I do not completely agree with the statement that the fast convergence of the simulations after the end of the assimilation interval indicates that other effects may influence the discrepancies. Nighttime and daytime ozone chemistry are very different. As mentioned above, one should check with other days or observation sites if the performed parameter changes are beneficial. But of course, other parameters could have an influence. The authors should mention possible candidates.

Additionally, as mentioned in the beginning: It should be discussed in how far this study gives valuable results for local CTMs in general or only for DRAIS, or only for a specific day simulated by DRAIS.

Language and other minor issues

1 Introduction
first line: "was carried out"

"Urban plumes are of special interest ...". I would assume that urban plumes are of special interest because of the sometimes high degree of pollution occurring there.

"Unlike other experimental sites ..." I don't understand what you want to say with this sentence. Maybe two sentences make things clearer.

"The urban plume is not influenced ..." Either "any other source" or "many directions".

Last sentence: "... uncertainties which probably cause discrepancies". Uncertainties can not cause discrepancies. Errors can.

2.3
"Figure 8 shows ... change in ozone production ..." Probably the authors mean the net production (?). This should be corrected here and in other places.

3 Sensitivity analysis
"The adjoint models therefore was developed ...". "Therefore" is related to what?

3.1
"The distance function decreases ...". When what is done?

3.2.1
"... NO is the most sensitive species ..." I admit, that it is a bit circumstantial to formulate correctly. However, not NO is a sensitive species, O3 is sensitive to NO emissions. The authors should correct this here and in the rest of the paper.

3.2.4
If there's only two important reactions the authors should mention them in the text and not only their indices.

4 Variation of relevant parameters
"It would be interesting ...". What does "would" mean. Partly the authors discuss this later.

5 Conclusions
"It is not surprising that the first five parameters are the most sensitive ones ..." This is probably not what the authors wanted to say.

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"However, their place in the ranking list ... could not predicted." By what?

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