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Atmospheric Chemistry and Physics Discussions

ACPD

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Interactive Comment

Interactive comment on "Emission rate and chemical state estimation by 4-dimensional variational inversion" *by* H. Elbern et al.

H. Elbern et al.

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We thank Ref. 1 for his/her constructive comments.
Prior to our response, we want to apologize for the missing figure reference and other failures in the very first paper version, due to overseen strange technical effects of our local implementation of the LATEX ACPD template.

This is our response:

General:

1) There are some editing needed. a) Most figure numbers do not show up in text; b)

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Figure 5 does not match its caption; c) Caption of Figure 6 is missing; d) pp18, $J_m in$ should be J_{min}.

a) This was a result of technical problems with the LATEX compiler. Figure numbers are now, as in later manuscript versions visible.
b) Figure 5 caption has now been adjusted to panel arrangements.
c) In the latest version, caption Figure 6 is not dropped out from the page.
d) This has been amended.

2) In this paper, assimilation time window is chosen as 24 hours. Whether this is long enough for the adjusted emission rates to have effect on predicted chemical fields is questionable. This has been demonstrated by O3 predictions in Figure 6. It is recommended that more explanation or discussion be given on this issue.

It is understood the referee means that the pure emission optimisation case (Fig. 6 bottom right panel, blue line) is to be considered by the remark, as the joint emission/initial value optimisation is satisfying. The ozone prediction following emission rate optimisation is unsatisfactory during the first day in the case of exclusive emission rate optimisation. Obviously, the three optimisation runs prior to the case of August, 9, had little beneficial impact so far in this mostly rural, low emission region, with interspersed towns.

We agree, that longer assimilation intervals allow for optimisation of slowly reacting VOCs, which are now only controlled by the emission error covariance matrix. However, due to the delayed ozone formation engendered by precursor emissions, given fixed initial fields, also a longer assimilation interval would not help to fully correct the simulation performance of the first 24 hours of simulation.

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The choice of the assimilation window has been taken as 24 hours, because this is the length of the diurnal profile of emissions, taken as strong constraint. With 24 hours it is already quite long, if compared with meteorological practice: ECMWF extended the window from 6 hours to 12 hours. While it is surely desirable to have long assimilation intervals, a couple of time limiting factors must be considered as well:

- The errors of the underlying models both the driving MM5 and the CTM must stay small enough during the assimilation interval for correct observation signal interpretation. As an example, slight shifts in wind direction and boundary layer height change due to phase errors of advected synoptic patterns clearly jeopardize correct processing of innovation signals in the critical regions.
- With increasing assimilation interval length the tangent–linear approximation underlying the variational approach looses validity, as a consequence of the highly nonlinear chemistry under photochemical conditions.
- With increasing assimilation interval length, the preconditioning of the minimisation problem becomes more challenging, as for example discussed in Chao and Chang, 1992.
- The computational burden quickly increases probably to an unaffordable extent, without gaining a reasonable improvement of predictive skills.

Tests with reduced assimilation interval lengths of about 14 hours, which were conducted to a 2 days period, indicate no substantial difference in emission rate factor estimates. Nevertheless, we adhered to the 24 h interval length because of the like design of the diurnal emission profile. On the other hand, we agree, that the optimal assimilation lengths must be further tested in practice, which will be compute intense. Presumably, a distinction between case study analyses and operational forecasts will be practical, including the identification and assessment of typical analysis errors due to too short assimilation intervals.

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Action: The discussion of the assimilation lengths is added to the text.

3). The results regarding the information content of various observations are of great interest. As we move forward in data assimilation the issue of what observations are most valuable is a key question. The results presented here show that the addition of a key precursor to ozone formation (i.e., NOx) did not improve the prediction skill. This is discussed in the paper and largely attributed to model resolution. Do you have results that might support this?

After introducing nesting techniques with adjoint modelling as part of 4D-var, there are presently studies under way at the research group of the authors, to systematically investigate assimilation performances with nested domains. A preliminary result can be obtained, for example from a survey paper Elbern and Strunk, 2005 (see http://www.ecmwf.int/publications/library/do/references/show?id=86890)

Indeed, by increasing predictive skills with increasing resolution, the formal interpretation given in the study under review, resting on the EKMA scheme, is corroborated.

Action: We shall add a related remark in the paper with reference, indicating first corroborative results.

Can you comment on what is the value of assimilation of satellite observations on the regional predictions?

Likewise, in Lahoz et al. (2006), section 2.4,

(http://www.cosis.net/members/journals/df/article.php?a_id=4938&FrameEngine=false) a first quantitative estimate of a single case study is presented, where GOME–1 tropospheric NO2 columns were assimilated. The preliminary results indicate only very moderate improvements. However, with increasing spatial resolution of satellite viewing geometry, significant improvements are hoped. This is presently under investigation.

W. A. Lahoz, A. J. Geer, S. Bekki, N. Bormann, S. Ceccherini, H. Elbern, Q. Errera, H. J. Eskes, D. Fonteyn, D. R. Jackson, B. Khattatov, S. Massart, V.-H. Peuch, S. Rharmili, M. Ridolfi, A. Segers, O. Talagrand, H. E. Thornton, A. F. Vik, T. von Clarmann, The Assimilation of Envisat data (ASSET) project, Atmospheric Chemistry and Physics Discussions, 6, 12769-12824, 2006.

(Now fully accepted and to be transferred to ACP)

Specific:

Remark:
1) pp.2, line 4: ", mapped to regular grids" It is not necessary to always map observation data to grid.Sometimes, it is impossible to do such a mapping, such as using the satellite column data.

Response: It would appear this is loose writing on our part. Surely, operator **H** needs not be invertible to map one–to–one between observation space and model space. What we meant is the entire data assimilation procedure as a mapping process between the combined model–observation space onto the model space.
Action: To clarify the text, we propose to make the following change, by replacing "'*mapped*"' by "'*analysed*"'.

2) pp.2, line 6: ", density, frequency" It is not clear what "density" means here.
The term density refers to the spatial coverage (density) of observation sites, frequency refers to the frequency of observations.
Action: We clarify the text by adding "'*spatial*"' to density.

3) pp.8, equation (9): It is better to indicate that Th, Tz, and Dx are operators that are

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performed with a half time step, unlike chemistry operator at a full time step.
Action: The text will be supplemented by mentioning the "‘half time step"’ for the transport and diffusion operators, according to the reviewer’s remark.

4) pp 11, equation (17): How is Ç0.69Ç picked in the equation?
Response: Considering the fact that observational information is restricted to the surface level, while imprecise climatological boundary values control the middle and upper troposphere, we estimate better model performance closer to the surface. Consequently, lacking more precise knowledge, the background error variances are set to 50 % at the surface and 100 % at model top, as described in the text. Equation (17) interpolates between the height levels by exponential formulation, thereby accounting for the roughly exponential grid spacing of the model height levels. Hence, with $0.69 = \ln(2)$, equation (17) can be rewritten as

$$\epsilon_{rel}(k) = \frac{1}{2}2^{\left(\frac{1-k}{1-k_{max}}\right)} = 2^{\left(\frac{k_{max}-k}{1-k_{max}}\right)}$$

Action: We propose to add this to the text.

5) Figure 3 and 2nd paragraph on page 14: How are the correlation between different emitted species estimated?
Response: Correlations have been estimated based on the emission inventory for polluter groups and statistics of emission strengths broken down into different sources.
Action: We propose to add this sentence to the text.

6) pp. 16, 2nd equation: It seems that (L/Delta x) should read as (Delta x/L).
The referee is correct. The formula will be amended accordingly.

7) Figure 4 is difficult to read.

The figure will be redesigned accordingly.

Interactive comment on Atmos. Chem. Phys. Discuss., 7, 1725, 2007.

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