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Interactive Comment

Interactive comment on "Ozone data assimilation with GEOS-Chem: a comparison between 3-D-Var, 4-D-Var, and suboptimal Kalman filter approaches" *by* K. Singh et al.

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General comments

This paper compares 3D-Var, 4D-Var, and suboptimal Kalman filter (KF) tropospheric ozone estimates based on ozone observations from the NASA Tropospheric Emission Spectrometer and the GEOS-Chem chemistry transport model. The produced analyses are evaluated on the similar lines of Geer et al., 2006. The novel aspects of this paper are:

- The first direct objective evaluation of global tropospheric ozone analyses obtained by the intercomparison of 3D-Var, 4D-Var and suboptimal KF assimilation solutions.
- The introduction of an original technique that propagates 3D-Var increments back to an equivalent initial condition, which provides a suitable comparison with 4D-Var.

This is a generally good paper which contains results of interest for the general chemical assimilation community. It is quite close to being acceptable in ACP as it stands. However, I would like to see some changes related to the discussion in parts of the paper, which will improve the paper if it is implemented. These changes are listed below:

Specific comments

p22264 / Eq. (21): The elements in the forecast error covariance matrix block (corresponding to each observation grid point) need to be squared.
p22268 / Fig. 4: More detail is needed in the discussion of the localized overcorrection in the mid west Australian region brought by the suboptimal KF system. Given the fact that 3D-Var and suboptimal KF processes are assumed to provide similar estimates, could you please explain in more detail why the overcorrection is visible in the KF solution and not in the 3D-Var one?. There are issues related to the difference in error covariance characteristics specified for the two assimilation schemes that could lead to such discrepancies:

- The forecast error variances at observation time $i+1$, in the suboptimal KF case, are constructed by transporting variances at observation time i as passive tracers, which is not the case in the 3D-Var process.

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- As used in this paper, the KF solves the same statistical problem as 3D-Var, but in observation space, then maps the solution to model space. This observation-space approach of KF uses a forecast error covariance matrix that differs from the model-space 3D-Var background error covariance matrix. The KF scheme used in this study is more comparable to the PSAS approach (Physical-space as Statistical Analysis System), which solves the analysis in the observation space.

- Neglecting spatial correlation (diagonal background error covariance matrix) would lead to giving too large weight to the background in the 3D-Var analysis. In order to compensate for that effect, the assumed variance of the errors should be increased.

- The J_{min} (cost function at the minimum) approach provides a diagnostic of the consistency of an assimilation algorithm (Talagrand, 2003). The error covariances are considered to be properly specified in the case when:

  $$E(\frac{2J_{min}}{N_{obs}})\sim 1$$

  Where E is the statistical average (expectation) and N_{obs} is the number of observations used in the analysis.

  In the case when $E(\frac{2J_{min}}{N_{obs}})>1$ the covariances are underestimated, and vice versa. If the authors have already produced this diagnostic, it may be useful to report the results of it in the paper.

- The χ^2 (chi-square) diagnostic can also be used as a self-consistency check of the specified error covariances for the KF assimilating system (Khattatov et al., 2000). For each assimilation analysis the value of χ^2 can be computed as:

  $$\chi^2 = (x^{obs} - Hx^f)^T(HBH^T + R)^{-1}(x^{obs} - Hx^f)$$

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Assuming that observation error covariance matrix R is known, and the Gaussian assumptions are considered appropriate, the statistics of χ^2 can be used as verification tools for the forecast error covariance matrix P^f. This latter is considered to be properly specified in the case when :

$$E(\frac{\chi^2}{N_{obs}}) \sim 1$$

In the case when $E(\frac{\chi^2}{N_{obs}}) > 1$ the covariances are underestimated, and vice versa. If the authors have already produced this diagnostic, it may be useful to report the results of it in the paper.

p22270 / Fig. 7 : Could you please explain why, in the longer assimilation case, the localized overcorrection in the mid west Australian region seems to be prominent in the 3D-Var solution and accentuated in the KF one?

Minor comments

p22249 / l1: to explore the role of of uncertainties (OF).
p22251/ l12: the characteristics 3-D-Var and 4-D-Var (OF 3-D-Var and 4-D-Var).
p22251/ l16 : Geer et al., 2006 PROVIDE (not PROVIDES) an intercomparison of STRATOSPHERIC ozone (not TROPOSPHERIC).
p22252/ l2 : The assessment of analyses generated through different assimilation systems IS (not ARE).
p22256/ l16-17 : Remove l16 and replace “AND” in l17 by “WHERE” .
p22259/ l6: The corresponding TES observation operator (3).
p22270/ Sect. 6.3 : It should also be mentioned in Sect. 6.3 that, in a 4D-Var analysis, error covariance propagation plays at least some part in explaining the differences between 3D-Var and 4D-Var.

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It would also be extremely useful for chemical assimilation community to compare 4D-Var with 3D-FGAT (First Guess at the Appropriate Time), a variant of 3D-Var in which the objective function is calculated by comparing observation values with the background at the relevant observation times. The 3D-FGAT scheme uses a more exact innovation vector than does standard 3D-Var, in which all observations over the assimilation window are compared to the same first-guess field. 3D-FGAT can be easily implemented by taking the adjoint model as the unit operator in Eq. (11) of the paper. The gradient of the cost function in 3D-FGAT should not use any explicit dynamics other than the trivial dynamics expressed by the identity operator. The increment to be added to the background state is, hence, constant over all the assimilation window instead of propagating it with a linear model. Therefore, it is possible to perform a direct comparison of the ways 3D-FGAT and 4D-Var use the observation information to constrain the model at the beginning of the assimilation interval.

p22274/ l17: The mathematical formula of the 3-D-Var equivalent initial condition $x_0^{e(3)}$ needs to be corrected.

p22276/ l24: the IONS datasets were (not WHERE).

References

Geer et al. (2006), The ASSET intercomparison of ozone analyses: method and first results, Atmos. Chem. Phys., 6, 5445- 5474, doi:10.5194/acp-6-5445-2006.

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Talagrand, O. (2003), A posteriori Validation of Assimilation Algorithms, in R. Swinbank, V. Shutyaev and W. A. Lahoz (editors), Data Assimilation for the Earth System. Dordrecht, The Netherlands: Kluwer Academic Publishers, 85-95.

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