

Interactive comment on “Diagnosing spatial error structures in CO₂ mole fractions and XCO₂ column mole fractions from atmospheric transport” by Thomas Lauvaux et al.

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General comments In this article, the authors use covariance filtering methods recently developed in the NWP data assimilation context and adapt them in the atmospheric transport framework. Their goal is to get a better estimation of the forecast error spatial structures for in situ carbon dioxide mole fractions and total column dry air mole fractions. I think that it is a very good idea to import methods from one domain to another, and I congratulate the authors for this effort.

I am not a specialist of atmospheric chemistry, so I will not be able to assess the relevance of the experimental setup used in this paper. In my comments, I will focus on the

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covariance filtering aspects, since the authors use the theory that I have developed for my PhD thesis. I think that some parts of the paper need major clarifications regarding the use and implementation of filtering methods. Detailed remarks are listed hereafter.

Authors: We thank the reviewer for constructive and helpful comments that improved the quality of this study.

Specific comments 1. I think that there is a mistake in the definition of the criterion $L(F)$ line 14. The criterion should be a scalar, so the transpose sign should be put after the first parentheses

Authors: The equations have been corrected accordingly. Thank you for spotting this.

2. I don't really understand why the authors assume that the dichotomy algorithm fails at converging if the filtering length-scale becomes larger than 750 km. Indeed, as shown in Ménétrier et al. (2015a), appendix C, the filtering length-scale verifying the optimality criterion for a homogeneous and isotropic filter always exists and is unique. As explained in section 8 of this paper, the value of this optimal filtering length-scale can be related to two ratios: $\hat{\sigma}$ the signal-to-noise ratio for the variance (related to the true variance values and the sample size), $\hat{\rho}$ the ratio between the variance signal and noise spatial variations length-scales (the noise length-scale being related to the forecast error correlation length-scale, see Raynaud et al. (2009))

If the optimal filtering becomes very large, leading to a constant value for filtered variances, it does not mean that the dichotomy algorithm is failing. It is a sign that the noise amplitude is too large compared to the signal variations and/or that the variance signal and noise length-scales are mixed. As a consequence, the filter prefers to filter out all spatial variations and keeps the mean value only (which might be the best option). I suggest a rewriting of the discussion about the convergence failures.

Authors: We have replaced the term “failure” by “convergence beyond our 750-km threshold” and clarified the description of the convergence. We set the threshold to

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750km assuming that length scales beyond that value correspond to filtering structures extending beyond our simulation domain of 1,600km by 1,600km, hence not filtering spurious noise as initially intended. The algorithm may converge to large values but such dimensions have no physical meaning. As the reviewer pointed out, these large values correspond to low signal-to-noise ratios, or to similarities between noise structures and true variance structures. Our initial terminology was incorrect because the filter does converge. The text has been modified through the entire paper and the terminology changed.

3. The covariance filtering theory leads to fractions of polynomials with factors $(N - 3)$ at the denominator, so 4 members is the absolute minimum ensemble size for this theory. I think that a 5-member ensemble is still too small to get significant results, and I would suggest to use ensembles of size 8-10 at least.

Authors: We now recommend 8 to 10 members in a more general case. The introduction and discussion sections have been updated accordingly.

4. For the localization of correlation functions, the Schur filters given by equations (9) and (11) are not positive definite functions, as mentioned in Ménétrier et al. (2015b). Thus, a fit of the raw localization function with a positive definite function is required before applying the localization. It seems that the raw localization function was used in this paper, which is problematic. Also, it is not clear how the spatial and angular average was performed to estimate the statistical expectations of equations (9) and (11) via an ergodicity assumption.

Authors: We agree with the reviewer that this step is currently missing. Considering that this study only looks at the filter to diagnose variances and correlations, we decided to skip the regularization for now, assuming that this part is critical when constructing the error covariance matrix out of the filtered variances and covariances. In a future study, we will regularize the solution before using our diagnosed error structures in an actual CO₂ flux inversion. We added some text in the last section to disclose that problem for

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future studies.

5. For Figures 8, 9 and 10, the small domains overlap, which makes difficult to see the functions shapes. It would be better to have separate boxes as in Figure 13 of Ménétrier et al. (2015b). Moreover, it would be more helpful to plot the localization functions, rather than the localized correlation functions.

Authors: Unfortunately, the overlap between towers is inevitable due to the distances between sites. To generate a figure similar to figure 13 of Ménétrier et al. (2015b), the map would need to be distorted with 7 separate blocks corresponding to the 7 measurement locations used here. Instead, to present more clearly the results of our study, we added some text with a reference to the figure 12 in which length scales are presented more clearly for each tower and for each day. "We present the localized correlation length scales for each tower and for each day in Fig. 12 (upper left panel). For both Center and Mead, length scales are noticeably larger than for the other towers and decrease rapidly until July 2nd, before converging back to the same values diagnosed for other measurement sites. The differences across towers suggest local differences in error correlations, even across the same region for a single day (up to 70 km across our sites). These differences correspond to the beginning of summer, when both weather and ecosystem fluxes vary rapidly especially in agricultural areas."

Authors: Related to localization functions, we did not include localization functions voluntarily to avoid confusion between error correlations and localization functions. This study aims at presenting the filtered error correlations for future applications, with less emphasis on the filtering method itself.

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