

Interactive comment on “Adjoint inverse modeling of a CO emission inventory at the city scale: Santiago de Chile’s case” by P. Saide et al.

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Answers and comments to referee N2

We appreciate your review. Your comments refer mainly to shortcomings in the algorithms to solve co-localization, simplifications regarding the use of the model in the inversion procedure. Also, you address the applicability of the L-curve method.

In following, we address one by one your comments, grouping them when suitable (in *Italics*).

Overall, we insist in the robustness of the algorithms (to solve co-localization and the L-curve method) and argue that the inversion method used is suitable for case of study.

C1233

The straight forward approach to solve this problem appears to be the specification of those off diagonal elements in the (multivariate) emission error covariance matrix B, which describe spatial correlations.

As mentioned in section 4.1.4, this is just one way to solve this problem, and maybe the most commonly used (see Page 6338, lines 23-24). However, there are several methods. The standard approach suggested by the reviewer is not the best approach for our case of study. In fact, the method we use gives better results than the standard or most commonly used approach (See Fig. 1).

Further, the effect to confine optimised emission rates to the grid cells with observations can be overcome by extension to spatio-temporal inversion techniques, which link cause (emissions) and effect (observed concentration levels) by modelling. It appears, that in this sense, the approach presented in this study could be regarded as a complexity reduced technique with simplifications from more complex algorithms.

If what you mean is that we should use the model on-line with the optimization routine, then we do agree. And in fact, this is exactly what we do. But instead of running the model every time that the iteration is done, the H matrix, which contains the spatio-temporal information, is pre-calculated using the model. This can be done because the model linear affine (page 6334, lines 17-20)

Also, pre-computing the H matrix result in simplifications and reduction of computing time. For the case of study, nothing is improved if the model is run inside the optimization. Moreover, it can be theoretically demonstrated that the results should be the same. This is a known fact, e.g. see Davoine and Bocquet (2007).

Abstract and Page 6339, beginning of 2nd paragraph, also to be considered intro-

C1234

duction of factor matrix F, page 6335: In particular, the central role of a proposed F factor matrix, to be multiplied with the background error covariance matrix, is pointed out. This method appears to be inspired by Issartel et al 2007, but is claimed as own development. The description includes elements of implementation, however, a mathematically rigorous optimality criterion and an associated algorithm to achieve this is lacking. The authors should add a proper description, justification and derivation of their method. Also the abstract, when addressing this issue, is unclear on what will be provided in the paper.

Issartel et al. 2007 shows a method for estimating the activity of a point source whose location is unknown. For this, they define a renormalization function that is computed through an optimization criterion. We tested this function for the case of study with bad results (Refer to the manuscript, page 6339 lines 8 -11). Then other types of functions were tested, finally obtaining the function presented in the manuscript (In page 6339 is explained how this function was found). Overall, we used an optimality criterion for the F factor to choose the norm used in Eq. (11). Different norms were tested for a synthetic run, and the one with best results was norm 1.

Thus, even though we recognize Issartel et al.'s approach, we tested several other normalization functions. So what we claim as a new development is that in a variational method we can apply a weighting or normalization function that resembles that of Issartel et al., but is constructed and applied differently. Part of the differences arises from the fact that we are dealing with a distributed source, often co-located with the observations.

The purpose of this paper is not to rigorously show the generality or some theoretical optimality of the proposed method. We simply present the development of a method that works better than others for the case of study in which co-localization of sources and observations hampers the ability to retrieve the optimal emissions. This is generally the case for methods solving the co-localization problem (e.g., Peters et al., 2005, Carmichael et al., 2008).

C1235

page 6331: Inflow boundary conditions are really zero, without any background values? If so, how is it justified?

Up-wind from Santiago de Chile comes mainly from the ocean, where clean air is found (in this part of the world). Since the background CO is really low ($\ll 0.1$ ppm), it does not affect the values found in the city, which mainly obey to local emissions

Description 4.1.1 : The description of the sensitivity matrix H calculation is unclear. Basically, the direct model calculates the forward sensitivity, and not the backward, as the adjoint of it, and hence both cannot serve the same purpose, (except perhaps for applications when linked by scalar products). The approximation of the adjoint by calculation of the wind field backward in time can be taken as approximation for the adjoint, but how this is finally used in an inversion algorithm, which basically needs both, the forward/tangent-linear and the adjoint, is not made clear. Also, the figure caption Fig. 7 does not help and should be reformulated accordingly.

When there is no chemistry involved the model can be completely replaced by its linear approximation (Eq. 1). Thus, in the inversion algorithm you only use the H matrix, and not the model (e.g., Davoine and Bocquet, 2007). In theory, for a linear tracer, the adjoint model is exactly the direct model after changing the sign of the winds and running backward in time, since turbulent mixing is self-adjoint. In practice, the validity of this is somewhat weakened by numerical and computational implementations (Davoine and Bocquet, 2007). However, in our case, as shown in Fig 7, this approximation is found to be suitable. Fig. 7 caption will be changed to: "Scatter-plot comparing direct and adjoint concentrations. Direct obs. are obtained running the model with the emissions to be optimized (x_b), and adjoint obs. are obtained computing H matrix through the adjoint applying Eq (1) with $y_0 = 0$ and $x = x_b$. Units in $\mu\text{g}/\text{m}^3$ "

C1236

Page 6337: The description of the L-shape method is insufficient. It should be noted that the quantities calculated with Eq. (10) are not error terms, as they are not the basis for calculating the error variances σ s obs/par, but the logarithms of inverse error covariance weighted squares of analyses-minus-background discrepancies.

To avoid the long name you propose (inverse error covariance weighted squares of analyses-minus-background discrepancies), we refer to the error in obs/par as the global term in the functional of Eq.(2), as stated just before Eq. (2). We will clarify this denomination, and yes the word "logarithmic" is missing in several sentences. This will also be corrected.

The plausibility of the result presented is difficult to assess. So, given reasonable estimates of R and B, the results of Eq. (10), prior to logarithm application, should be of order of the number observations (trace of the unit matrix in observation space) and of order of the number of horizontal grid cells (trace of the unit matrix in surface grid space) (for further explanation, if needed, see a posteriori validation papers from Talagrand 1998 (ECMWF proceedings) or div. papers of Desroziers et al.) .

This would be the case if we used Eqs. (4) and (5) for estimating the optimal emissions. However, we use the functional of Eq. (2) with positive constraints, as explained in section 4.1.3. This is one of the reasons why the L-curve approach is used, since it allows handling the violation of the Gaussian assumption over the parameters being estimated.

The plausibility of the values of σ (from Eq. (9)) given in Figure 8, and the final result of $1.4e+7$ should be demonstrated by means of discussion of observation and emission rate errors.

C1237

If we had those error estimates, and we were confident about those we would certainly use them. However, this is not the case and we use instead the L-curve approach. In page 6337, lines 2-10 is explained that due to lack of information this is not possible. The range of values is so broad that either the improved inventory is too close to the initial guess or it is completely different. This is why the L-curve approach is chosen, since it finds a balance between both terms of the functional J as explained in section 4.1.2.

Further, the related Figure 8 axes should explicitly express logarithmic scaling, as is used.

We are plotting the logarithms of the errors and not the errors, thus the scale is logarithmic (as plotted) but there is a mistake in the axis labels since the word logarithm is missing. This will be fixed.

Page 6340, first paragraph of 4.2: Typically, the complexity of variational data assimilation algorithms, is not dominantly dependent on the number of observations and not controlling the computing time dominantly.

As stated earlier, what we do is to pre-calculate the sensitivity matrix. These computations depend linearly on the number of observations since we use the adjoint (for every observation we perform a model run, see details in section 4.1.1).

Also the description of a reduced inventory should be reformulated, to make it clearer.

We do agree. It has been reformulated.

C1238

Page 6342, 1st line: what is the “time average of the morning/afternoon hour” ? Please make clearer.

It is temporal mean of the emissions only considering morning hours (6 to 12 AM). This is in the next paragraph (line 7). The order will be changed to make it clearer.

References

Carmichael, G.R., Sandu, A., Chai, T., Daescu, D., Constantinescu, E., Tang, Y., Predicting air quality: Improvements through advanced methods to integrate models and measurements, *Journal of Computational Physics*, Volume 227, Issue 7, Pages 3540-3571, ISSN 0021-9991, DOI: 0.1016/j.jcp.2007.02.024, 2008.

(The rest of the references are in the Manuscript)

Interactive comment on *Atmos. Chem. Phys. Discuss.*, 9, 6325, 2009.

C1239

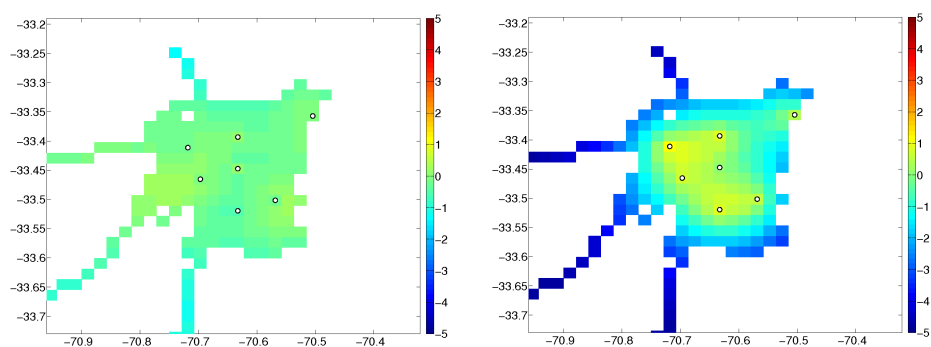


Fig. 1. Synthetic simulation results using correlations with a radius of influence $r=2.5$ over B matrix (right) and using the factor proposed in the manuscript (left). Difference between real and optimized EI

C1240