

Interactive comment on “Direct Inversion of Circulation and Mixing from Tracer Measurements: I. Method” by Thomas von Clarmann and Udo Grabowski

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We thank the reviewer for the insightful and thorough comments which certainly will improve the paper. In the following we have included the reviewer's comments in *italic face*. Our replies are printed in normal face.

General comment:

The paper presents a method for deducing atmospheric circulation (wind field) and mixing parameters from trace gas measurements by inversion of the continuity equation. In a first step, the mathematical framework is defined and explained. Second, the

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method is applied to idealized tracer fields and to MIPAS satellite measurements (in the “proof of concept” section 5), to show that the inversion indeed results in reliable velocities and diffusivities.

Deducing information about the circulation from measurements, without involving information from models, is a great challenge in atmospheric sciences. This paper seems to contain an important contribution to reach that goal, what renders it definitely publishable and of great interest to a large readership of ACP. However, I have two major points which the authors need to assess before publication. First, the paper is not easy-to-read and the presentation quality needs improvement – otherwise I feel that the paper will fail in addressing a large readership. Second, I have some concerns about the so-called “proof of concept”.

We thank the reviewer for this encouraging general comment. We are confident that we will be able to improve the presentation quality. The specific comments of the reviewer are of great help here. With respect to the issue of the “proof of concept”, please see our reply below.

Major comments:

1) Presentation and Notation:

Overall, the paper is overloaded with detailed formulae, but lacking motivating and explanatory paragraphs. In their own words (P2, L33), the authors aim to avoid “that the reader does not see the forest for the trees” but, in my opinion, there are still too many trees around. For instance in section 3, there should be a clear motivation at the beginning, why the derivatives (which are calculated in the following) are needed and what the matrix notation means.

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We agree that some sentences of motivation of certain steps will be helpful and we will include some.

After that the equations (15-26) could be nicely combined into one single equation-array (similarly in section 4, starting with equation (37)).

The sentences between the equations are meant to guide the reader through the forest of equations and to motivate what each single equation is good for. We think that without these explaining sentences the general criticism that there are too many equations and too little explaining and motivating text would be even more applicable.

Concerning all formulae, writing $X; x; \mu; \dots$ for mixing ratio instead of vmr would help to increase readability.

The problem with our paper is that it is interdisciplinary, addressing the communities of remote sensing, inverse theory, atmospheric modelling etc. The suggested notation would clash with the conventions in some of the communities mentioned. For example, x is usually the independent variable in inverse theory, and μ is often used as expectation value. In our own context, we need variable x later for the combined state vector. Thus, we are inclined to stay with the self-explaining variable name.

Moreover, while many steps in the calculation are written in detail (like taking derivatives), at some points I was not able to understand the derivations in detail. One such example is the matrix notation in equation (27). First, a clear motivation should be given why this matrix notation is advantageous...

The matrix notation has been chosen because with this the formalism can be expressed in a much more compact manner. We will include a note on this.

and what it means (this is the heart of the paper).

We agree that this is the heart of the paper and deficiencies in clarity at this point would be detrimental. On the other hand, the meaning of the terms is explained in the itemization after Eq. (27). We have decided for the following to make this part more transparent: We will include a figure which will illustrate which block of the D-matrix operates on which components of the initial state vector to produce which components of the final state vector. In the itemization after Eq. (27) we will then refer to this visualization. We are inclined to follow this approach because we think that a pure verbal description would make the paper more tedious to read, would add unnecessary length, and would not necessarily add clarity.

Second, I did not succeed in understanding the dimensionalities of the quantities involved. As the authors state, the D-matrix is build from three submatrices of dimensions $K_0 \times K_0$ (I_K), $K_0 \times 2K_0$ (W_i), and $J_0 \times L_0$ ($D_{\rho;nom}$). Therefore, the D-matrix has dimensions $(2K_0 + J_0) \times (3K_0 + L_0)$, which is, as far as I can see, not consistent with the vector it is acting on. Please check the dimensionalities again and explain clearly what equation (27) means.

The D-matrix is not block-diagonal, that means, the dimensions of the sub-matrices it is formed of cannot simply be added to give the total dimension. Some of the sub-matrices act on the same components of the input state vector. As written above we will visualize this.

Equation (35) caused me similar problems with understanding. Please explain clearly where it comes from.

Here the same explanation holds as sketched above.

The appendix is, in my opinion, not necessary. It just presents a recalculation of the existing literature. I would recommend to reduce such recalculations, but to add explanations at the critical and new steps of this paper (e.g., around Eqns. 27/35). If the authors want to keep that part, it could be moved to the supplementary material.

What has been published as an appendix in the discussion paper was initially just an internal document to help ourselves to better understand the issue of eddy transport and why zonal averaging can cause additional transport and mixing components. It was initially not foreseen for publication. It was not part of the initial submission. The other reviewer, however, requested a more thorough discussion of these issues, and due to that, we have decided to include this. Due to the lack of original content, we have decided to include it as appendix only. To provide this as a supplement might indeed be a good compromise. **Since inclusion of this was triggered by a comment in the other access review, a recommendation on this issue by the other reviewer would be highly appreciated.**

2) *“Proof of concept”:*

In my opinion, section 5.3 does not really present a “proof of concept”, as promised by the title of section 5. The method is used to deduce velocities and diffusivities from tracer measurements, but the true underlying circulation is not known. Therefore, this case is no proof that the inversion method yields the correct result.

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This is why in Section 5.1. and 5.2. we test the method using idealized cases where the functionality of the components can be easily judged.

I think, for a true “proof of concept” the circulation and diffusivities must be known before and need to be reproduced by the method. Section 5.2 points into this direction, but is exclusively descriptive. The optimal “proof of concept” would be to have a 2D-model based on equations (3-4) with idealized velocities and diffusivities, and to invert the resulting trace gas distributions. At least, the cases described in section 5.2 should be explained in more detail and related results should be shown in the paper.

We have chosen the title “proof of concept” in order to avoid the more ambitious term “validation”. While validation aims at providing evidence that the system provides the correct results in a quantitative sense, the claim of a proof of concept is, to our understanding, much weaker. A “concept” is little more than a quite general idea, and a “proof of concept” just shall generate confidence that it is worthwhile to pursue these activities, that there is no evidence that the concept leads inevitably into a blind alley etc. Actions towards validation of this method have been initiated, including comparisons with models etc, but these are far beyond the scope of this methodical paper.

In reply to this comment, we will take the following actions:

1. We will add some text where we describe what the proof of concept is meant to be, in order to avoid to raise false expectations.
2. We will present some of the studies undertaken under 5.2.

Specific comments:

P2, L1ff: Another source of uncertainty when deducing mean age from SF_6 is related to the fact that the tropospheric increase is not strictly linear (see Garcia et al., 2011,

JAS).

We agree that non-linearity of tropospheric SF₆ is an issue. However, this non-linearity in the tropospheric SF₆ time series is considered in the work of, e.g., Stiller et al (2012) or Haenel et al. (2015). These authors use an iterative scheme to infer the age. As first guess, they use the age directly inferred from the SF₆ mixing ratio. Then, they calculate the age spectrum for this initially guessed age, convolve the (non-linear) tropospheric time series with this age-dependent age spectrum, infer a correction, and iterate until convergence. Thus, the only remaining uncertainty in this context is the uncertainty of the age spectrum. However we agree that not every reader might be aware of this method, and we will add a note on the non-linearity issue.

P2, L7: To my knowledge, in models usually the surface layer is used as a reference, not the upper edge of the TTL. Please clarify.

There seems to be some disagreement in the modelling community. At least, in a review of a paper by Stiller et al., 2012, the reviewer insisted that the age of air is defined relative to the time of entry into the stratosphere, and the reviewer was not at all happy with our reply that an age defined like this is an empirically void theoretical quantity. But if the models indeed use surface as reference, then even better! Then their age indeed is a quantity with empirical content. We will reword the text accordingly.

P18, L11: How robust are the deduced velocities and diffusivities with respect to the choice of initial value for the iteration. Please give some quantitative estimate.

In a constrained retrieval, where the initial guess is set equal to the a priori field, there are generally two possible mechanisms for a dependence of the result on the initial

guess.

1. **The effect of the constraint:** The solution of a constrained inversion always has a tendency to be pulled towards the a priori field, or, in our case with 1st order Tikhonov constraint, the field gradients are constrained to those of the a priori field. Our a priori constraint is chosen as zero velocity throughout. Since the resulting field gradients deviate largely from this initial guess and resemble those of the expected velocity fields, it is evident that the inversion is able to find a solution which is far away from the initial guess and is not overly constrained by the a priori assumption.
2. **Non-linearity and possible secondary minima of the cost function:** The observed convergence rate indicates an almost linear inverse problem; thus, no such related problems are seen. We have experienced that problematic cases regularly end up in non-converging iterations rather than converging to different results and are thus easily sorted out.

Our results provide the smoothest field of velocities and the smallest mixing coefficients which are still consistent with the measurements. Any change of the a priori assumptions must have an impact on the results. How large this intentional dependence is, is fully user-controllable by adjustment of the regularisation strength.

P20, L7: How can the residual be small for SF_6 if no chemical sink is included in the calculation? Is the sink effect absorbed in the transport terms, or is a significant sink only existing above the upper boundary for the calculation?

The problem with the sink in Stiller et al. (2012) is, that age-calculations are sensitive to the accumulated decomposition since the air has left the troposphere. In our case, only the decomposition during the finite time-step of the calculation can contribute,

because the atmospheric state at the beginning of the time step already is depleted in the trace gases. For SF₆, the major sink is indeed above the altitude range under consideration.

P20, L13: “Velocities are roughly consistent with mean ages...”. Some misinterpretations in the past arose from relating mean age simply to the stratospheric circulation. However, mean age is known to be controlled by circulation and mixing (e.g., Neu and Plumb, 1999; Garny et al., 2014; Ploeger et al., 2015). So please discuss carefully what you mean here with “consistent”.

We emphasize the attribute “roughly”. This statement is not meant as a quantitative assessment but is meant to say that there is no obvious major contradiction between our results and our current knowledge on stratospheric mean age of air. We will change the text towards a more careful wording.

Technical corrections:...

We are grateful for the thorough reading of the manuscript and will carefully apply the corrections.

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