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Interactive comment on "An extended Kalman-filter for regional scale inverse emission estimation" *by* D. Brunner et al.

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We would like to thank Lori Bruhwiler for the constructive comments and for the positive and encouraging remarks. Below we present a point-by-point reply (referee comments in italics)

General comments:

One suggestion I can make that may make the paper slightly more general, is that a short discussion be included on the applicability of the technique to gases that have natural or agricultural fluxes (e.g. CO2, CH4, N20).
This is a good point. We are confident that the method is readily applicable to CH4 for which surface sources in Europe are greatly exceeding surface sinks (we already

performed some tests for CH4) and most probably also for N2O. We are currently starting a project for estimating CO2 sources and sinks and plan to evaluate the approach presented here against an established (CarbonTracker type) inversion. It is obvious that for CO2 some adaptations will be required, in particular to account for the fact that fluxes can be negative (hence taking log(emissions) will not make sense) and to account for strong diurnal variations in its sources and sinks. CO2 with its diffuse natural sources and sinks in addition to anthropogenic emissions is challenging and we believe that the quality of a CO2 inversion is ultimately more strongly depending on a careful design of covariances (e.g. correlations in the behavior of different plant/land surface types) rather than on the specific inversion approach. An advantage of our approach in comparison with an Ensemble Kalman Filter as used in CarbonTracker is that the transport simulations need to be performed only once (to estimate the source receptor relationships) whereas the source estimation can be done independently. The sentence on P29198 line 3 starting with "In this study .." will be replaced by: "In this study we present an emission estimation approach generally applicable to long-lived or weakly reactive trace gases with only positive surface fluxes (emissions), i.e. trace gases with negligible deposition/uptake at the surface. The method is demonstrated for halocarbons which are measured quasi-continuously at only few sites in Europe, and the ability to invert emissions on a country-by-country basis is explored." The first sentence in the conclusions section will be replaced by: "An inversion method based on an extended Kalman filter was developed to estimate regional scale emissions of passive or weakly reactive trace gases with positive fluxes from the surface to the atmosphere. For gases like CO2, which do not only have large emission fluxes but also significant uptake at the surface, the method would have to be modified to incorporate negative fluxes and to account for the strong temporal variability of surface fluxes."

Specific comments:

For minor points not mentioned explicitly below we followed the recommendation one to one.

29196, L15-16 - Would the emissions be reported to the "Kyoto Protocol"? Or the UNFCC? Isn't the Protocol an agreement rather than an entity that one would report to?
Agreed, sentence changed to "reported to UNFCCC in the framework of the Kyoto Protocol".

29196, L25 - "integrate" or "represent" rather than "comprise".
Changed to "integrate"

29205, L11-13 - It would be useful here to have a short discussion of why the ln(e) is used. This is because many readers might read this paper with the idea of estimating CO2 emissions.
We added the following sentence: "The logarithm is taken to constrain emissions to positive values but it also ensures that residuals (differences between modeled and measured values) closely follow Gaussian probability distributions, a prerequisite for successful Kalman filtering. Note, however, that this limits the applicability of the method to trace gases with only positive fluxes (emissions) and would not be valid for species like CO2 with important negative fluxes."

29206, L13 - If D is the linear model, then why is it sparse? I don't understand this.
The matrix D_k is sparse because our linear model is a very simple one. For a persistence model the matrix is simply the identity matrix. As explained in the text further above and in Eq. (2), the matrix D_k is in our case essentially diagonal with only a few off-diagonal non-zero elements. Maybe "sparse" is not a good term for this type of almost diagonal matrices, but in our case it is not exactly a tridiagonal matrix either. We changed the sentence to: "Since the matrix D_k is almost diagonal with only few off-diagonal non-zero elements, we compute the few non-zero terms in Eq.5 explicitly rather than performing the expensive full matrix multiplication."

29208, L14 - Could correlated errors arising from transport errors be accounted for in the R matrix? This would de-weight the influence of the observations, of course.

The stations considered are sufficiently distant (Mace Head, Jungfraujoch) from each other that we can safely assume that transport errors at the two sites are uncorrelated. In general, however, the matrix R would indeed be the right place to describe such correlations. After the sentence "As usual, the matrix R_k is chosen to be diagonal assuming no correlation between errors at the different stations" in Sect. 2.4 we will add the sentence: "Note, however, that in the case of a dense measurement network with stations located close to each other it might be necessary to include off-diagonal elements in the design of R_k to account for correlated transport errors."

29209, L24 - How was the correlation length scale chosen? Would it be the same for all emissions? For example, what if emissions from use as blowing agents is very local, but emissions from leaking refrigeration is more distributed?
The length scale was set to 500 km for all emissions. Although this selection is quite arbitrary it is in the same range as correlation length scales used by other authors in similar studies (e.g. Thompson et al., Atmos. Chem. Phys., 11, 3443-3458, 2011). We admit that this is currently a weak point. Further optimizing the error covariance matrices depending on the species considered will certainly be a point we will particularly emphasize in our future work.

29210, L10-14 - Does the iteration become necessary because of the non-linearity arising from the use of ln(e)?
No, the iteration was only applied for the reasons mentioned in the manuscript. Primarily, to be able to eliminate the time lag which unavoidably appears in a Kalman filter which, different from a smoother, only accounts for past observations. In addition, the tests with synthetic data suggested that a solution with 3 iterations on average better recovers the original emissions than a solution after a single run. With more years of data and more realistic a-priori information, however, it will likely become beneficial to perform a single forward and backward simulation only (2 iterations). The ultimate goal is to apply a Kalman smoother and assimilate each data point only once.

29211, L14-20 - Is the parameter describing the transport error in the footprint the

same for both sites? Wouldn't this differ between Mace Head and Jungfraujoch?
Yes. We will add the following lines at the end of Section 2.5 to point out this limitation of the current setup: "A limitation of the current setup is that the transport error ρ_{SRR} is optimized over all stations simultaneously. In future studies we will investigate possibilities to better account for the varying ability of the transport model to describe the meteorology at, and the transport to, individual sites while at the same time keeping the optimization problem manageable."

29213, L1-4 - How are the aggregation errors computed?
The total emission X_c of a country is obtained as the scalar product $X_c = \mathbf{z}_c^T \cdot \exp(\mathbf{x}^e)$ where z_c is a country-specific mapping vector of the same dimension as the emission field. The elements of z_c represent the fraction of the grid cell located inside the country. The relative aggregation error is now obtained as the difference $(X_c^{\mathsf{red}} - X_c^{\mathsf{ref}})/X_c^{\mathsf{ref}}$ where X_c^{ref} corresponds to the total country emission obtained with the high resolution (reference) inventory (Fig. 3a) and X_c^{red} those from the reduced grid. In the column "with sea" in Table 1 the elements of z_c are calculated slightly differently: For grid cells partly covered by land and partly by sea, the sea fraction is proportionally attributed to all countries contributing to the land-covered fraction of the grid cell. This information will be added in the revised manuscript.

Interactive comment on Atmos. Chem. Phys. Discuss., 11, 29195, 2011.