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Interactive Comment

Interactive comment on "A two-step scheme for high-resolution regional atmospheric trace gas inversions based on independent models" *by* C. Rödenbeck et al.

Anonymous Referee #2

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General Comments

This manuscript presents a recipe for the combination of global- and regional-scale transport simulations and inversions for CO_2. As regional inversions with higher temporal and spatial resolution become more and more important, methods to couple such inversions with the global background are needed. The authors present a new approach to this problem, which, however, appears to have some weaknesses. These weaknesses don't invalidate the recipe suggested, but I have doubts whether they outweigh the advantage of less work to prepare models.

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Interactive Discussion

Discussion Paper

Specific Comments

For the assessment of this manuscript, I found four main questions to be relevant, for which I am offering my comments:

1. **Is the mathematical framework valid?**

   (a) In Eq. 3 it is not explained whether variables are Reynolds-averaged or not. As such averaging is a precondition for any practical solution on a large domain, I presume that variables are thought to represent suitable means. Then, however, the turbulent diffusion term is missing, which is relevant at least for the vertical dimension in the boundary layer.

   (b) Authors introduce a 'regional mixing ratio field $c^{reg}(x,t)$' which is said to be a solution of Eq. 1 with Eq. 4 as boundary condition.

   It should be noted that, before numerical representations with corresponding simplifications are introduced, there is only one field c, and looking at a subdomain does not create a new field c^{reg}.

   It should also be noted that boundary conditions for the continuity equation should be given in the form of fluxes (von Neumann boundary condition), not in the form of fixed values (Dirichlet boundary condition), as it is done throughout this paper.

   It should be noted that the boundary condition as given in Eq. 6 for the contribution from insided the DoI, namely $c_{nh}^{reg} = 0$ is unrealistic and certainly wrong for outflow borders.

   (c) The authors say: 'Since the transport operator T is linear in the mixing ratio, the solution within the DoI can be represented mathematically as the sum of two unique components:
   (1) a homogeneous solution with no fluxes in the DoI but which matches the boundary conditions on ∂DoI, and

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(2) a non-homogeneous solution which has zero boundary conditions, but which is subject to the fluxes in the DoI.'

This is not correct. The solution to an inhomogeneous linear PDE can be obtained as the sum of the general solution (i.e., fulfilling the initial and boundary conditions!) of the homogeneous equation, and any particular solution to the inhomogeneous equation. The splitting made by the authors into two parts fulfilling different boundary conditions does not correspond to this standard procedure.

(d) The authors say: 'The homogeneous solution $c_{hom}^{reg}(x,t)$ is generated by any pathways from fluxes outside the domain and transported into the domain across the boundary (O–I pathways), or by any pathways that started inside the DoI, temporally left the DoI, and re-entered the DoI later across the boundary (I–O–I pathways).'

Apart from the fact that the wording 'solution ... generated by ... pathways' is awkward, the second part of the statement is misleading. Let us assume that 'pathways that started inside the DoI' should mean 'mass that is injected into the system by sources inside the DoI'. (If a 'pathway' were a trajectory, how could it start anywhere? That would be contrary to the continuity condition.) If such mass leaves the DoI, it is lost as there is no feedback from c_{hom}^{reg} to c^{glob}, and $c^{reg}(x,y) = 0 \quad \forall (x,y) \notin$ DoI. Only if we look further into section 2.4, we discover that a first set of calculations will be carried out on the global domain with the coarse model, and the mass that was introduced into the system from inside the DoI can then become a part of the regional $c_{hom}(x,t)$ through the boundary condition.

This situation would in principle call at least for an iteration, repeating step one with DoI fluxes obtained by step two, etc. At least an iteration needs to be tried in a representative setting to find out how big its effect would be.

From this it follows that the method is, even after correction of the formulation of the boundary conditions, only an approximation. However, the authors don't make it really clear where their approximations are, and generate a false impression of mathematical accuracy.

2. **How well has the quality of the method been established?**

   There are a number of factors that will obviously affect the quality of this approximative method: numerical procedures and resolutions, size of the domain and its location with respect to the main fluxes and flow patterns (this is addressed in the manuscript to some extent), degree of aggregation in the resultant fluxes.

   (a) The tests were carried out with TM3 as both global and regional model, and with grid spacings of (x-direction) 8° for the global and 4°, or, resp., 1.8° for the regional simulation. If we compare this with the motivation presented by the authors in the introduction, we can observe that the regional-scale test simulations were carried out with a resolution that is effectively a good global-model resolution, and targeted regional resolutions would be much finer. It remains open how the system would perform with such more realistic settings.

   (b) The authors mention that they would like to use Lagrangian models for the regional simulation. However, given the very different nature of Eulerian and Lagrangian models, it is not at all clear how they would be interfaced in the sense of the two-step scheme, as the recipe is presented in terms of Eulerian description only.

   (c) It should be noted that all comparisons presented between the fluxes of the 'benchmark' and the two-step procedure are for highly aggregated fluxes only, and grid-by-grid results are not shown, although they should show much clearer any problems, especially boundary-related ones. As the authors state that the inversion aims a producing gridded fields ('pixels') of the fluxes, this seems to a serious shortcoming.

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3. **How valuable is this method compared to the alternatives?**

   I would see the following alternatives:

   (a) A nested or zooming global model, as already mentioned by the authors, with (more) proper handling of the boundaries. In the case of a nesting approach, two-way nesting would clearly be desirable. I admit that it is more work, but many nested transport models have already been written, including the TM5 model. Thus, what is the value of running TM3 in this approximative setting?

   (b) For me it is not clear why the forward run with the manipulated coarse model to calculate $\Delta c_{mod,nh}$ is necessary. Couldn't this term just be skipped in Eq. 13, and the fluxes insided the DoI be dermined as $\mathrm{f}_1 + \mathrm{f}_2$, so that f_2 would be a correction to the first guess obtained with the global model? That would be even more simple than the suggested procedure.

4. **Is there enough substance to warrant publication as ACP research article?**

   The proposed method is best characterised – also by the authors themselves – as a recipe. In my opinion, it does not have a very solid theoretical base, but it is 'reasonable' and the authors have shown that it works well enough—at least under the conditions of their tests. These tests, however, are far from being general. Alternative solutions including global models with two-way nesting capability are available and appear more attractive. This paper does not present substantial new findings. Thus, it should—if it is found publishable in ACP—be published as *Technical note*.

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Minor comments

1. p 1732, l 8: *input . . . is the . . . ratios.* mismatch singular/plural

2. The wordings *(non-)homogeneous contribution*, *(non-)homogeneous mixing ratio*, etc. are kind of sloppy, and at least for me they appear to make the text more complicated to read.

3. There is no information on the driving meteorological fields.

4. There is no information on the vertical resolution of the models in Table 1.

5. The only reference for TM3 given is an internal report without URL. No information on the numerical methods used in TM3 are given.

6. The first item in the list of Appendix A is not phrased in a generally understandable form. For example, it is hard for me to imagine what is meant by *spatial elements cut at the boundary*. If this explanation is deemed necessary, maybe it would be better to include the formulae. This example also shows that the method really depends on the discretised set-up.

7. p 1744, l 8, *step-2 inversion*: step 2 of the inversion would be more clear. Same on line 12.

8. In Figures 3 and 4, a different scale for the fluxes is used in each panel (belonging to some region). However, these scales are not oriented at the amplitudes of the fluxes. All figures should either use the same axis endpoints, or alternatively, axis endpoints should correspond to the minimum and maximum of the respective figure. In any case, the endpoints should be chosen so that the curves shown are not clipped.

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9. In Figures 6 and 7, we see features that look like data gaps. Such gaps must not be connected with lines. Also, it should be said whether values are hourly, daily, weekly ... If they represent means for periods long enough to be visible on this scale, then a step (bar) curve would be more appropriate. Finally, the panels are too small to be of much value and need to enlarged, Figure 7 also in the vertical scale.

Interactive comment on Atmos. Chem. Phys. Discuss., 9, 1727, 2009.

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