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Geoscientific
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Discussions

Interactive comment on "The Lagrangian chemistry and transport model ATLAS: validation of transport and mixing" *by* I. Wohltmann and M. Rex

I. Wohltmann and M. Rex

ingo.wohltmann@awi.de

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Dear Paul,
thank you for taking the time and reviewing our manuscript. Your suggestions were very helpful for improving the paper.

Important notes

- I discovered a bug in the model code shortly after submitting the paper (the sur-

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face pressure needed for the calculation of the model level pressures was not read in correctly). Although the effects are rather small in the stratosphere, I decided to do the model runs again. Most figures show slightly different results now. Since changes to the results were small, text and conclusions did not change, with the exception of some values of diffusion coefficients, which are slightly larger now.

- On request of the other referee, the manuscript was restructured. Section and Figure numbers in the following refer to the old manuscript.

Major comments

- 1. You are certainly right that it would be desirable that the ATLAS method of triangulation would also be feasible for higher resolutions and that the restriction to coarser resolutions leads to some disadvantages (like a less realistic representation of the diffusivity of a single mixing event and the impossibility to do detailed studies of filaments and small-scale mixing). However, there are good reasons to run models also at these coarser resolutions, like doing decadal long-term runs including chemistry.

  At these resolutions, the ATLAS method would be preferable to the CLaMS method and, as we agree, it would certainly be much better than the Eulerian approach. So I think it is fair if I claim that the approach is superior for these coarser resolutions.

  I have added some discussion of the unrealistic behaviour of mixing at coarse resolutions to Section 5.5. I also added additional remarks to the abstract and the results section that the mixing algorithm is only applicable for coarse resolutions.

  It is made very clear in the paper that the approach only works for coarse resolutions (just before using the word “superior”, page 717) and it is admitted slightly

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later that this restriction is “unfortunate”. There is only one other place where the word “superior” appears, in this case it refers to the objective fact that the values of ε in Fig. 8 are lower for the ATLAS method than for the CLaMS method. It is not claimed anywhere that our model performs better than CLaMS in high resolutions. So I think the description is sufficiently balanced.

Moreover, it is obviously not true that no comparison between model and experimental data is shown for coarser resolutions. In fact, most Figures (8, 9, 10, 11, 14, 15) show results for all resolutions. The examples in Figure 5, 6, 7 are only shown for 50 km, but this is something that you have done analogously in your papers. With good reason: Showing additional data from other resolutions would increase paper length and it makes sense to show the best examples available.

It is also not true that the model validation was only done in CLaMS mode. All relevant plots show both triangulation approaches and both approaches are discussed in the text.

It is also sufficiently clear where results of the CLaMS or ATLAS methods are discussed. E.g. for Figure 5, it is obvious that it uses the CLaMS triangulation and there is no claim in Sect. 5.3 that the quality of the results is due to the ATLAS method.

- 2. The text of the corresponding paragraphs was changed somewhat to make the discussion clearer. It is a valid objection that $\varepsilon = 0$ and $\gamma = 1$ do not imply perfect agreement. I have added some discussion of this to the end of the paragraph about ε and γ.

  I did not significantly extend the discussion beyond this. Although I would find it interesting to discuss some of these issues in more detail, I have to make a cut somewhere to keep the paper readable. The paper is already very lengthy and I think at some point this would go beyond the scope of a model description paper. Instead, I will give some discussion here in my reply.

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I agree the intensity of mixing influences roughness and vice versa. In fact, they are so highly correlated that you could approximately predict one quantity from the other quantity. This relationship is also sufficiently described in the manuscript. It is specifically the *additional* patchyness and the *displacement* of filaments (which one could see as two different effects) by errorneous wind fields or the discretization, which are better separated by the new definition of the parameters. Indeed, I make the assumption here, that, to first order, the new definition of ε is not affected by these effects, and therefore gives a clearer separation of these effects between γ and ε. Since these effects would influence where the minimum of ε is situated, they would also influence the choice of the mixing parameters, e.g. possibly the diffusivity would be set to higher (or even lower) values than in reality. The main statement in the text is that these specific effects can be better separated.

Two quantities which are highly correlated and interconnected can still be very different quantities in reality (e.g. nobody would say said Arctic temperature and chemical ozone depletion are the same quantity and you can easily define them separately, nevertheless they are highly interconnected and correlated). In this sense, I think it is justified to speak of a better separation and definition although mixing and roughness correlate.

It is claimed in the paper that ε only includes the effects of "mixing intensity". There is no stringent physical or mathematical definition of "mixing intensity", "chaotic advection" or "roughness" in the paper to keep the paper readable. This may lead to some subtle differences of what is meant by these terms, but I think to most readers the meaning will be sufficiently clear.

If I would e.g. define "mixing intensity" appropriately, say, by the mean effective diffusion coefficient (at the location of the flight path), or equivalently by the average number of mixing events a parcel experiences in a given time and their strength (given by the parcel distance), I could probably proof that in good ap-

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proximation ε is only affected by "mixing intensity" (every mixing event is a linear interpolation between two points on the tracer-tracer mixing curve, the more often the interpolation happens and the more distant in tracer-tracer space points are, the more the curve is lifted to the concave side, etc.). Of course, "roughness" would influence that, e.g. by influencing the difference of mixing ratios of two mixed points, but if I would assume that effective diffusion is constant along the flight path and that the additional filaments have the same mixing ratios as the "old" ones the effect would be small ("displacements of filaments" as such would not change ε anyway).

All these arguments get more difficult due to the differences of mixing in reality and in the model. E.g. in reality chaotic advection is coupled to the strength of mixing, since e.g. more stretching would trigger more gravity waves. However, in the model, the wind field (and hence the chaotic advection) is prescribed and we can introduce any "mixing intensity" on top of it, which may be very unphysical.

The discussion in the paper is normally only based on the (mathematically sound) definition of the old and new ε and γ. In addition, I tried to phrase things carefully (e.g. "we *try* to put effects into γ").

In summary, I think I do not suggest that these definitions are stronger than it would be justified in the paper.

- 3. I agree that the estimated diffusion coefficients will probably be more realistic in higher resolutions. I have added some discussion of this in the paragraph describing Fig. 13. It is never claimed in the manuscript that the ATLAS triangulation mode would be useful for comparison with in-situ data, so I regard this issue as settled. I don't think further discussion about limitations is needed, since these were very clearly stated in the paper, see also major comment 1.

  I do not agree that nothing can be learned about atmospheric diffusivity from coarser resolutions and the ATLAS mode. While there are certainly limitations by

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the unrealistic diffusivity of single mixing events and missing the fine filaments, there is still some information in the bulk diffusion coefficient and the mixing curve in tracer-tracer space.

I would like to stress here, that at coarse resolutions, these are no particular limitations of ATLAS, these are limitations of CLaMS also. And there is good reason to use these coarse resolutions for long-term runs. Even if ATLAS and CLaMS are not performing particularly well here, we can be sure that Eulerian models would perform even worse. I think that is the important point.

Minor comments

- *Title:*
  Added "advective" to the title to make it clear. I would not agree that the usual connotation is that transport includes mixing. Most people will think of long-range advective transport here and not of microscopic random processes.

- *page 710, par 15:*
  This should better read "Mixing ratios of inert tracers are conserved by design" (to avoid confusion with changes by chemistry). The important point is not that mixing ratios *are* positive by design (this is due to the initialization, not the transport algorithm), but that they *stay* positive by design. There is now a short note below the list that the Lagrangian derivative is conserved in absence of local sources on request of the other referee.

- *page 715, par 5:*
  The paragraph has been rewritten (as requested by the other referee), which solved this issue.

- *page 717, par 20:*
  You are correct. However, this is discussed in detail in the paper (Fig. 13 and

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accompanying discussion) and it is shown that the additional diffusivity is small in most cases.

- *page 718, par 5:*
  You are right, several details are missing here by purpose. I decided to skip some information because the paper was already very lengthy. I have now added an appendix describing some details of the 3-D triangulation.

  I did not include one of the issues raised here in the appendix since I think it is sufficiently clear from the paper: It is not intended that the method returns the "true" 3-D neighbors. The final neighbors are no approximation at all of the 3-D neighbors. The purpose of the method is that the triangulation returns the neighbors in a layer centered on the original parcel, with the definition of the layer and all other aspects being unchanged in comparison to the CLaMS method. The 3-D triangulation is only an intermediate step with no particular physical or geometrical importance for the method. As noted in the text, the "cloud" of parcels could also be obtained by looking for all points below a critical distance to the original point, were it not computationally too expensive. Likewise, all points outside of the mixing depth Δz need to be cut, since the 3-D triangulation can easily produce neighbors with a large vertical distance to the original point, which is unwanted behaviour.

- *page 718, par 10–15:*
  Since the approach is not used in the end, this is not discussed in detail in the manuscript. I will explained it here in more detail.

  Imagine the model is initialized such that the mean horizontal distance in a (CLaMS Δz) layer is r_0 and the mean vertical distance $\Delta z/2$. Now imagine we introduce the same number of points again such that the mean parcel distance in the layer is reduced to $r_0/2$. If we would now triangulate in 3-D, the neighbors of a particular point would be vertically closer on average to the original point as

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if we would triangulate in 2-D with the given Δz. We would miss some points close to $\pm\Delta z/2$ since the triangulation would find some points vertically closer to the original point that are more optimal for the tetrahedrons for geometrical reasons. These points are not necessarily the horizontally nearest neighbors in the complete layer. In effect, we would have introduced an additional "layer" of points, which shields points that are vertically more distant. In turn, this hinders the merging of points in the r_- step, since the average horizontal distance of neighbors will be larger than it would be if we considered all points in the original Δz layer. The r_+ step will then add additional points, which introduce new artificial "layers" and so on. The problem is that the "layer" "visible" to a particular point gets vertically smaller in each step, so that the number of points increases without a decrease in the horizontal distances of the nearest neighbors. This cannot happen if the layer depth Δz is fixed.

- *page 718, par 20:*
  I would like to improve the description, but it is difficult to figure out what you mean if you don't specifically describe what details are missing.

- *page 718, par 25:*
  Paragraph has been removed.

- *page 719, par 25:*
  Do you mean that the determination of the next neighbors is spoiled by the random number or do you mean that adding the random number offsets the lower diffusivity that is obtained from the ATLAS triangulation method? The first issue is easy to solve: Since the random number is added after the determination of the next neighbors, it does not interfere with their determination. The second issue is discussed in detail in the paper (Fig. 13 and accompanying discussion). It is shown here that the additional diffusivity from adding the random number is negligible in most cases.

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- *page 720, par 20:*
  As far as I can see, the citation is correct.

- *page 721, par 5:*
  Strictly speaking, you are right. The statement is only correct for r_0. For the sake of simplicity and readability, and since it is mentioned in the next sentence that an initial separation r_0 is used, I would like to keep the wording.

- *page 722, par 5:*
  Figure 16 has been moved. The maximum is correct. The number of parcels is decreasing in the course of the model run for intermediate values of λ_c. That means that the mean parcel distance increases.

- *page 723, par 1:*
  You are correct, there is only one. The sentence originally referred to the list starting at page 714, line 20. But of course, there is just one pressure coordinate system with two different wind options. Changed the text accordingly.

- *page 723, par 10:*
  Done.

- *page 726, par 5:*
  What do you mean by "numerical diffusion of a linear interpolation"? Diffusion can either be interpreted as a process acting on some scalar field (i.e. concentrations), as given by the diffusion equation, or as a random walk of a number of particles. It cannot act on a "linear interpolation". If it is meant that diffusion acts on a linear function here, it would not be possible to estimate the diffusion coefficient from that: A linear function does not change under diffusion.

  I think there is a problem due to discretization here, both in time and space. The question should be: Given the mixing ratio of the newly created point, the distances of the old points, and the mixing time, what diffusion coefficient, what

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(continuous) variation of the mixing ratios between the points and what variation of diffusion with time would be compatible with the mixing ratio we inserted? E.g. assume that we have rather different mixing ratios in the two points we mix, because the large-scale advection created two neighboring filaments and assume the continuous variation between the points is a step function at first, with the step at half distance. Diffusion would now act to smooth out the step with time, but the value half the distance between the old points would always be the mean of the mixing ratios of the old points (i.e. linearly interpolated), regardless of the diffusion coefficient. Hence, we cannot estimate the diffusion coefficient in that case! Neither could we if we assume a linear function as the variation between points. Hence, if we try to estimate the diffusion coefficient this way, we run into problems.

Eq. (8) can also be interpreted differently: In a normally distributed cloud of particles (say in the z coordinate) with standard deviation σ (this is the solution for the diffusion equation for a delta function as initial condition after a finite time and σ is a function of the diffusion coefficient and time, see Eq. (3)), the mean distance between parcels is $\Delta r = \sqrt{2}\sigma$. That is, if Δt and the diffusion coefficient are given, we can estimate the mean distance. Likewise, we can estimate the diffusion coefficient of an *ensemble* of parcels from their mean distance and Δt, if they would come from a point source. The weak point here is of course that the parcels are evenly distributed. But it is really difficult to come up with an equation without any strong assumptions in it.

- *page 729, par 5:*
  Changed.

- *page 734, par 20:*
  The equation is correct. The dependency on the observed values is in the function $\hat{h}$. I have added a superscript "obs" to make that clear. You can interpret the method as looking for the modeled point in tracer-tracer space and then go-

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ing down or up along the vertical axis (that is, along m_j^{model} until you meet the curve $\hat{h}$, which is fitted at the observations). I added a Figure with a sketch of the method (also on request of the other referee).

- *page 739, par 10:*
  Changed.
- *page 739, par 25:*
  Added reference.
- *page 740, par 5:*
  Would like to keep the wording.
- *page 741, par 0:*
  Changed.
- *Figure 2:*
  Replaced magenta by orange. Added "view from above" to caption.
- *Figure 8:*
  Changed the second occurence in the caption. The word "mixing mismatch" is used in numerous other locations throughout the paper as a shortcut for "difference between the observed and modeled tracer-tracer relationships". I don't think it makes sense to replace it everywhere.
- *Figures 11 and 12:*
  Moved to an appendix.
- *page 738, line 11:*
  Typo discovered by myself: It should read 150 and not 100.

Interactive comment on Geosci. Model Dev. Discuss., 2, 709, 2009.