Geoscientific
Model Development
Discussions

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

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

Important note

- We discovered a bug in the model code shortly after submitting the paper (the surface pressure needed for the calculation of the model level pressures was

not read in correctly). Although the effects are rather small in the stratosphere, we 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.

Major comments

- *First major point:*
  ATLAS is a new model that was developed from scratch and has no program code in common with CLaMS. We have added a comment in the introduction. Basically, the module concept and the mixing algorithm (that is, the general program work flow) are taken from CLaMS. All information needed to develop the model was taken from the CLaMS publications.

- *Second major point:*
  For the actual validation, the curves are *not* extended by additional values from other flights. This is stated on page 735, lines 7–8. The curves were only extended with other data in tests to show the validity of the approach. The tests were not used in the validation. We added an additional comment to the paragraph.

- *Third major point:*
  We agree that the paper is quite complex and lengthy. We will happily include your specific suggestions and clarifications to make it more readable. In addition, the manuscript was shortened considerably (the overall length did not decrease due to some additional requested paragraphs). We did not follow a very few suggestions of moving sections, since some sections build on each other and have interdependencies. We hope the order of the paragraphs is a good compromise now. More information is given at the specific comments.

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Specific comments

- *First specific comment:*

  – *Abstract, line 4–7:*
    We would like to leave the sentence in the abstract, since it is an important motivation for the paper.

  – *Introduction to basic concepts:*
    We added a paragraph at the start of the introduction giving a definition of numerical diffusion and explaining why Eulerian approaches usually suffer from numerical diffusion.

  – *Why is Lagrangian transport mass conserving by design?*
    While this is generally true for most simple Lagrangian models (by the usual definition of the air parcel as an entity consisting always of the same molecules), it is *not* true for our model (neither is it true for CLaMS, since the reason lies in the basic algorithm). In our model, *mixing ratios* are conserved by design (that is, the variable containing the mixing ratio is simply not changed during the trajectory run). The mass of the parcel may change: The horizontal density of parcels is constant (as a function of altitude) if measured in a layer of the extent of the vertical mixing depth Δz. If now Δz is approximately constant with altitude, an air parcel always occupies a constant volume. From that, it follows that the mass of a single air parcel is roughly proportional to pressure (due to the ideal gas law). The loss of mass of an uprising parcel is balanced by the creation of new parcels in the r_+ step, since there has to be a divergence in the horizontal wind field somewhere for continuity reasons. Likewise, a descending air parcel will be merged with other parcels in the r_- step, increasing its mass, in a convergence. This will not always be true for single parcels (e.g. since the

wind fields of the analysis may violate the continuity equation), but it will be approximately true in a statistical sense.

– *Why is computing time independent of the number of transported species?* Added a comment in the introduction. In an Eulerian model, a transport equation has to be solved for every single species in every grid cell. In a Lagrangian model, the transport equation has only to be solved once for every trajectory, only changing the coordinate values, but not the mixing ratios, since the Lagrangian derivative of the mixing ratios is always zero in the absence of local sources and sinks, in contrast to the Eulerian derivative.

• *Typical values:*
Since typical values are given in the sections with the results, I would like to leave the text as is to keep it more readable.

• *Section 2 and 3:*
Sections 2, 3 and 4 have been combined into a new Section 2 named "Model description". The text has been shortened. Order of paragraphs in new sections 2.3.3 and 3.2 has changed for more consistency. Other specific points of this comment:

– *Further I would ask the authors to provide more details about the model features:*
We included some more information about the model features, but we tried to keep this section relatively short. It was not our intention to give a complete model description here and to give more than the information relevant for the following discussion. We think that would overly increase the length of the paper.

– *Implementation of the troposphere:*
We think the information given in the paper is sufficient, given that the paper

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focusses on the stratosphere. We will give some additional information here. As stated on page 712, line 2, only a basic troposphere is included. That is, there is no special treatment of the troposphere at all. Air parcels are driven by the wind fields in the same manner as in the stratosphere. Since ATLAS is a Lagrangian model, no special treatment of the surface is needed. If the winds are correct and the trajectory time step is sufficiently small, air parcels will avoid obstacles automatically (if not they will be deleted). As stated on page 14, line 13–15, several components needed for a realistic representation of the troposphere are missing. One may also add a boundary layer parameterization to the list.

– *Choice of the mixing time step:*
As noted on page 721, line 8, the mixing time step has to be optimized by comparison with observations like the other parameters. In practice, there are some constraints on the mixing time step: Too short time steps are computationally too expensive and too long time steps destroy the neighbor relationships due to the non-linearity of the flow. This limits practical values to about 6 to 24 hours. Added a paragraph with some discussion of this to Section 4.3 (now 2.3.2).

– *Which time steps are implemented?*
As stated in the discussion paper, page 714, line 17, the time step is freely configurable (The only constraint is that the mixing time step is a multiple of the trajectory time step. Since that is rather obvious, we think this information can be omitted).

– *Which integration methods are implemented?*
In the moment a simple Euler scheme (1st order), an implicit iterative trapezoid rule (2nd order) and a 4th order Runge-Kutta scheme. We do not think it is necessary to give this information in the context of this paper. It does not add any insight.

- *How are the boundary layers defined?*
  The upper boundary layer contains all air parcels between the upper boundary and one mixing depth Δz below the upper boundary. The lower boundary layer is defined analogously. Added a sentence to the paragraph.

- *What happens to air parcels outside the model domain?*
  Parcels outside the model domain are deleted. Added a sentence to the paragraph.

- *Why should it not be possible to interpolate species?*
  Interpolation is accomplished by triangulating the old parcel positions and looking for the tetrahedron a new parcel is contained in and interpolating by barycentric interpolation to the new parcel. If there is no enclosing tetrahedron, this is not possible. This is typically the case if voids appear at the upper or lower boundary due to the large-scale motion (e.g. downward motion by the residual circulation at the upper boundary). Added a sentence with the above example to the paragraph.

- *Section 4:*
  Text has been shortened. Specific comments below.

  - *Last paragraph on page 718:*
    Skipped.

  - *Vertical clustering:*
    I found it fairly difficult to come up with a sketch that visualizes the problem better than the text describes it. Therefore I did not include a sketch.

  - *page 717, line 15–23:*
    Deleted large parts of the paragraph. It was actually very redundant.

  - *Section 4.2:*
    Moved as requested.

– *Section 4.5:*
  I would like to keep the paragraph at this place. It gives some information that is helpful for interpreting the results in Section 5 (now 3), like the formal dependence of the diffusivity on r_0 and λ_c.

- *Section 5:*
  See specific comments below. Text has been shortened.

  – *Restructure Section 5:*
    The paragraphs about the diffusion coefficients were turned into a new section as suggested. The section with the definition of ε and γ was not moved (new Section 3.4). Instead, I moved the paragraph in the introduction (new Section 3.1), which introduces ε and γ, to the new Section 3.4 and replaced the paragraph by a short table of contents of Section 3. This should also solve the problem.
    I would like to keep the order of the subsections, since moving the section with the definition of ε and γ in front of the sections with the model setup and examples would have the disadvantage that some things, like the figures showing the tracer-tracer correlations would not have been introduced yet. I have renamed the name of the last subsection 3.5 from "Results" to "Validation results".

  – *More tuning than validation*
    I changed the title of the new Section 3 to "Validation and tuning".

- *page 734, line 14:*
  Added a Figure showing the two different methods.

- *page 739, line 3–9 and Figure 11:*
  Moved into an appendix (with Fig. 12). I think it would not be fair to claim that our

method of calculating ε anf γ is more robust and not to proof that this really is the case. Therefore, I would like to keep the figures.

Minor comments

- *page 710, line 18:*
  Added SLIMCAT as an example.

- *page 710, line 26:* Changed.

- *page 713, line 22:*
  Since this sentence is in an introductory section and is my best attempt of a short summary of what is explained in more detail later, I would like to keep the wording, although it may be not very concise. The density I am thinking of here is the number of air parcels per unit volume (and not the number density of the air in molecules per volume). Strictly speaking, this quantity is not conserved, since it changes with time (see discussion of model resolution). Note again that it is more or less constant in the vertical (measured in units of the mixing depth Δz), which means that an air parcel represents a smaller mass at lower pressure.

- *page 713, line 23:*
  You are right. Changed the text somewhat. My intention was to say that apart from introducing mixing into the model, this procedure ensures that we get a homogeneous distribution of points, which is benificial for interpretation of model results and interpolation to some position.

- *page 713, line 26:* Changed.

- *page 714, line 10, page 716, line 2, page 716, line 8:*
  Added some detail to the definition of r_0. Added "initial" to make more clear that resolution will change with time. Added note that the initial resolution r_0 and r_0

from the mixing parameterization are set to identical values. We think that the definition of r_0^{eff} and other parameters is sufficiently clear.

- *page 717, line 14:*
  For resolutions < 150 km, memory consumption during the triangulation is the limiting factor (it does not work even with 16 GB). In a test with 150 km resolution, $\lambda_c = 3$ per day, 10 mixing steps and 16 processors the overall running time for the global layer approach is about 6700 s, with the calculation of the neighbors taking about 50% of the time (3000 s). The local layer approach takes 3400 s, with the calculation of the neighbors taking only 120 s.

- *page 718, line 2:*
  From Eq. (5), $\Delta z \approx r_0/125$ in the lower stratosphere, so it is typically a few kilometres.

- *page 718, line 5:*
  It is extremely unlikely that this happens and there are no precautions in the code to catch these cases to save computing time. Technically, the triangulation routine from the Qhull library ignores one of the duplicate points in this case.

- *page 722, line 1–2:*
  As stated in line 6, the number of air parcels (and the resolution) does generally decrease.

- *page 724, line 24, page 728, line 1, page 729, line 5, page 729, line 7, page 730, line 2, page 730, line 3:* Changed.

- *page 730, line 5:*
  In the stratosphere, either the potential temperature or hybrid coordinate are natural coordinates, since air moves along isentropes in good approximation. The hybrid coordinate has the advantage that we do not need to care if we include parts of the troposphere in the model domain.

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- *page 730, line 15–16:*
  It ranges from 10^4 for 300 km to 10^7 for 50 km. Added a sentence to the paragraph.

- *page 730, line 19:*
  I am following CLaMS notation here for consistency.

- *page 730, line 28:*
  In fact, this simple question is surprisingly hard to answer. The fact that the number of air parcels decreases is only an empirical observation with no mathematical theory behind it. During model development, I tried several modifications to the original CLaMS algorithm, and to my surprise, almost all of these modifications were not stable in the sense that either more parcels were deleted than added in every mixing step or vice versa and no steady state was reached. Changes like introducing a few parcels more in the merging step by not merging to only one parcel or using a 3-D triangulation directly would lead to a catastrophic growth (as mentioned on page 718, line 9–17). I suppose several facts like the properties of the atmospheric flow (e.g. continuity) and the properties and geometry of triangulation play a role here.

- *page 733, line 8:*
  I cannot figure out what you mean. It is written correctly in the manuscript (with r).

- *page 733, line 10–20:* Shortened.

- *page 734, line 2:* Changed.

- *page 737, line 16:*
  Since the results for γ are discussed later in the section, I think it is less confusing to leave the sentence as is.

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- *page 737, line 17-19:*
  It is not. Mixing is very low in our model if optimized by observations, and the small change in the observed tracer-tracer relationship over such a long period of time just reflects that. Slightly changed the wording of the sentence.

- *page 737, line 24, page 738, line 14, page 738, line 27:* Changed

- *page 738, line 28:*
  You are right. The case that there is no spurious noise in the wind fields and no discretization of the data is hypothetical. Slightly changed the wording of the sentence.

- *page 740, line 6–8:*
  There is no contradiction here. It depends on λ_c if it has an impact (and is necessary) or is negligible. Changed the sentence accordingly.

- *Figure 2:*
  Replaced magenta by orange.

- *Figure 3:*
  Improved the figures by moving the red lines in the background and making them less prominent. I tried several combinations of number of air parcels and marker size, and this is the best visualization I could find. The clustering is best visible if you zoom in a little bit. Note also that the lines of highest parcel density are curved for the ATLAS method (higher at the tropics), but at constant potential temperature for the CLaMS method (highest density is slightly above the red lines for the level boundaries).

- *Figure 5:*
  I think headings are unnecessary. They would only repeat information from the axes labels.

- *Figure 6, Figure 7*
  Added headings.

- *Figure 8:*
  Added line.

- *Figure 16:*
  Moved figure between Fig. 3 and 4.

- *page 738, line 11:*
  Typo discovered by myself: It should read 150 and not 100.

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