

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

Anonymous Referee #1

Received and published: 29 July 2009

General comments:

The paper presents the new global stratospheric CTM ATLAS with full Lagrangian transport. The basic approach is similar to the Lagrangian CTM CLaMS, but ATLAS includes an improved, less diffusive mixing algorithm. In a case study the mixing parameters of the model are optimised by a comparison with aircraft measurements. Furthermore, new estimates for the vertical and horizontal bulk diffusion coefficients in the stratosphere north of 60° are provided. Although the paper is an important contribution to the modelling community and deserves publication, it needs major revisions before being published.

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I have three major points of criticism: First, the new model ATLAS is based on or at least very similar to the Lagrangian CTM CLaMS (e.g. Lagrangian transport, basic mixing approach, limited to the stratosphere). From my point of view it is not quite clear whether ATLAS is really a new model or whether it is a further developed version of CLaMS. For example, in Section 3 the authors state that the trajectory module is based on the parallel trajectory code used in Wohltmann and Rex (2008). How does this code compare to CLaMS? In this respect I would ask the authors to clearly comment on what has already been part of CLaMS and what is new or has changed compared to CLaMS. The paper concentrates on the dynamical part of the model, making the model description somewhat incomplete as the chemistry scheme is missing. However, presenting the overall model including chemistry would overly increase the length of the paper. So I hope the companion paper on the chemistry module will be published soon.

My second point concerns the determination of the validation parameter ϵ . I agree with the authors that it makes sense to use the shape of the mixing curves instead of point-to-point distances between model and observations. However, I am a bit confused about the treatment of “outliers”, i.e. modelled methane values which are outside the range of the observations and therefore not used in the analysis. This procedure sounds a bit like cheating to me. Please clarify: Why is it necessary to extend the mixing curves with additional data from other flights? Which flights are used for the calculation of ϵ ? Do you compare single flights with the respective model simulation or do you use all available data together? What would you have done without the third or the eighth flight? Is ϵ really an all-purpose measure?

Finally, the paper is rather complex and the presentation should be improved as it is often difficult to follow. The paper covers several different topics, starting from a technical model description, mixed up with a discussion of different approaches (e.g. determination of next neighbours), ending up with a description of new diagnostics and a model validation. To be honest it took me more than a day to read the whole paper. Some parts of the paper I had to read several times, and some of them are still unclear to

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me. I have several suggestions and questions for clarifications that I think will further improve the paper and make it more accessible. After a revision taking the comments into account, I recommend to accept this paper for publication in GMD.

Specific comments:

- Abstract, l 4-7: You may put this sentence into the introduction. Generally, I suggest to include a short section into the introduction explaining the basic concepts of Lagrangian and Eulerian transport. For example, what is numerical diffusion? Why do Eulerian approaches suffer from numerical diffusion? Why is Lagrangian transport mass conserving by design? Why is computing time independent of the number of transported species?
- When talking about resolution, time step or number of air parcels the authors may give some examples or typical values, e.g. p 710, l 25; p 712, l 5/6; p 713, l 9/10;
- Section 2 and 3: You may combine both sections to an overall model description. I also suggest to include the basic description of the mixing algorithm (Sect. 4) into this section. Further I would ask the authors to provide more details about the model features, e.g. the implementation of the troposphere, the choice of the mixing time step. Which time step and integration methods are currently implemented? How are the boundary layers defined? What happens to air parcels outside the model domain? Why should it not be possible to interpolate tracers and chemical species from the old parcel position to the new parcels (p 716, l 7)?
- Section 4: In general, this sections provides a lot of detailed information, and I am not sure whether all this information is really necessary. I would ask the authors to carefully revise this section, concentrating on the main features of the mixing algorithm and reducing redundancy. For example, last paragraph on p 718: Is the approach for very high resolutions already implemented in the model? If not, I suggest to skip this paragraph or move it to a discussion or outlook section.

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Maybe an appendix would be another possibility.

Sect. 4.1: It is not quite clear to me why air parcels tend to cluster vertically. A little sketch might be helpful. p 717, l 15-23: I suggest to include this paragraph to Sect. 4.2. This might reduce the redundancy of this section.

Sect. 4.2: You may move this section behind Sect. 4.4.

Sect. 4.5: To my opinion this section is not part of the mixing algorithm. Therefore, I recommend to move this paragraph to a new discussion section on the vertical and horizontal bulk diffusion coefficients (see below).

- Section 5: This section is again rather complex. It includes a description of the model set-up, some examples from the model runs, a more general discussion and description of the two diagnostic parameters, results for γ and ϵ for different model resolutions and mixing intensities, and finally a general discussion on diffusion coefficients. All these different topics are combined in a section called "Validation", whereas it is more a "tuning" of the mixing algorithm than a "validation". First of all, I suggest to re-structure Sect. 5, starting with the description of the measures γ and ϵ , followed by the model set-up and determination of the best mixing parameters. Furthermore, I recommend to add a new discussion section dealing with the calculation and comparison of the vertical and horizontal bulk diffusion coefficients.
- p 734, l 14 whole paragraph: A schematic plot illustrating the analysis of the mixing curves might be helpful.
- p 739, l 3-9 and Fig. 11: From my point of view the authors may skip this figure and the related discussion. It does not provide important insights. Omitting this figure would further help to clarify the overall structure of the paper.

Minor comments, technical corrections:

- p 710, l 18: You may add some examples of CTMs.

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- p 710, l 26: Chemistry Climate Model (CCM)
- p 713, l 22: Is the density of air parcels really constant?
- p 713, l 23: Avoiding voids and crowded regions is the same as keeping the density of air parcels constant, isn't it?
- p 713, l 26: "... of McKenna et al. (2002) and, shortly recapitulated, ..."
- p 714, l 10; p 716, l 2; p 716, l 8, etc: Please explain your symbols. What is the difference between r_0 and r_0^{eff} ? A list of used symbols might be helpful.
- p 717, l 14: Only for interest: How much more expensive is the local layer approach than the global layer approach?
- p 718, l 2: typical values of Δz : Is there any rule of thumb?
- p 718, l 5: "ignoring the vertical coordinate": What happens if two air parcels have the same horizontal position and differ only in the vertical coordinate?
- p 722, l 1-2: Does the total number of air parcels increase or decrease during a model run?
- p 724, l 24: "... of 1 km and and a horizontal ..."
- p 728, l 1: "has to be tuned" instead of "has to be used"
- p 729, l 5: "distinguish between the two effects:" ?
- p 729, l 7: "... and hence has has an effect ..."
- p 730, l 2: "ALIAS and Argus measurements are ..."
- p 730, l 3: "Wherever possible, ..." ?

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- p 730, l 5: Why do you use the hybrid coordinate? Please explain.
- p 730, l 15/16: How large is the total number of air parcels for different model resolutions?
- p 730, l 19: I suggest to use Δt_{mix} for the mixing time step.
- p 730, l 28: Why does the number of air parcels decrease?
- p 733, l 8 and following: erroneously/erroneous
- p 733, l 10-20: This paragraph is very redundant and should be shortened.
- p 734, l 2: "... clear separation ..."
- p 737, l 16: You may add a comment that switching off mixing is not an option for optimising γ .
- p 737, l 17-19: This sentence seems to be taken out of context.
- p 737, l 24: CLaMS
- p 738, l 14: include "(see Fig. 8, right side)"
- p 738, l 27: minimum of ϵ ?
- p 738, l 28: To my opinion it is always necessary to find a compromise in optimising γ and ϵ .
- p 740, l 6-8: This summary sounds a bit strange. Does the random vertical coordinate have an impact or is it negligible? Please clarify.
- Fig. 2: magenta and red colours are hard to distinguish

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- Fig. 3: From the scatter plots I cannot identify any clustering of the air parcels. Either the number of shown air parcels should be reduced or the scatter plots should be skipped.
- Fig. 5, 6, 7: Headings would be helpful, e.g. Fig. 6, upper left: "Nearest model neighbour", upper right: "Average of the first neighbours".
- Fig. 8, right: An additional line at $\gamma = 1$ might be helpful.
- Fig. 16: This figure is already discussed in Sect. 4.3 and should be moved to the front between Fig. 3 and 4.

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