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Interactive Comment

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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Review of the paper:

The Lagrangian chemistry and transport model ATLAS: validation of transport and mixing written by I. Wohltmann and M. Rex

General:
The manuscript presents a new Chemistry Transport Model ATLAS, in particular formulation and validation of the Lagrangian transport. The model design mainly follows

the ideas and concepts used in the existing and well-documented model CLaMS. Because the numerical code of ATLAS is completely independent of the CLaMS code and some new physical and numerical ideas were applied both for the formulation and for the validation of the model, ATLAS contains new aspects which are worth publishing. In particular, the following points are the key new aspects of the paper:

- ATLAS reproduces in a an independent way the main features of CLaMS and, consequently, supports the original ideas and confirms the advantages of the Lagrangian transport (low numerical diffusivity, small-scale structure like filaments can be reproduced, transport barriers are better preserved,...)
- A new 3D method of the next neighbor determination is used in the low-resolution transport studies. This method has some potential to improve the layer concept of 2D triangulation implemented in CLaMS.
- The diagnostic parameters which allow optimizing the mixing scheme in CLaMS are re-formulated. In particular, the re-formulation of the roughness parameter γ contains some advantages compared to the formulation described in the CLaMS-related papers. Also the new definition of the mixing parameter ϵ contains some new interesting aspects.
- The discussion of the bulk diffusivities as derived from the experiments and from the Lagrangian simulations (Figures 14 and 15) gives some new quantitative insight into the quality of (Lagrangian) transport.

However, these new aspects, in particular the last 3 points, prompt some additional questions (major points of this review) which have to be addressed before this paper can be recommended for publication:

1. The use of the 3D triangulation certainly increases the number of air parcels with correctly determined next neighbors. However, this method is too time consum-

GMDD

2, C193–C199, 2009

Interactive Comment

ing and thus cannot be applied for spatial resolutions better than 150 km. This unfavorable scaling hinders the applicability of ATLAS for high spatial resolutions, i.e. for resolutions where the numerical diffusivity of one mixing event is becoming comparable with the physical diffusivity. Thus, such projects as reproduction of mixing lines measured with in-situ instruments (see conclusions), are only possible in the CLaMS-mode of ATLAS (i.e. using the CLaMS concept of staggered layers and 2D triangulation). On the other side, there are some places in the manuscript where the "superior" mixing scheme of ATLAS with less numerical diffusivity than in CLaMS is discussed. This is true for the low resolution ATLAS runs where no comparison between the model and experimental data were shown. So slightly exaggerating one may say that the model validation of ATLAS was done in CLaMS mode but the model advantages are described in the ATLAS mode (that were not validated in the manuscript because e.g. small-scale structures are not resolved). Here, slightly more balanced description would be desirably.

2. The optimizing of the mixing parameters slightly differs from the original procedure formulated in Konopka et al, JGR, 2004. Whereas the definition of the γ parameter quantifying the roughness of the time series was significantly improved, I have still some doubts with respect to the diffusivity parameter ϵ. Here the authors assume that both effects, i.e. the effect of the diffusivity and the effect of the chaotic advection on transport can be separated (i.e. γ measures only the ability of the model to reproduce chaotic advection and ϵ measures only the ability of the model to reproduce the mixing). However, in the real atmosphere these both effect are interrelated, e.g. roughness depends on mixing and mixing depends on the chaotic advection. Even if the presented definitions of γ and ϵ are justified, they are not so strong and stringent as this manuscript currently suggests. Furthermore, the relations $\epsilon = 0$ and $\gamma = 1$ do not implicate a perfect agreement between the simulated and observed time series. This is also not the case with

GMDD

2, C193–C199, 2009

Interactive Comment

the definition of ϵ given in Konopka et al, JGR, 2004 but there are fewer degree of freedom compared to the definition of ϵ proposed in this manuscript. Here a more detailed and critical discussion of these arguments is expected.

3. The effective diffusivites derived from the model and discussed in Figures 14 and 15 are something misleading. In particular, a model with a horizontal resolution of 300 km and with only few mixing events scores like a model with a very small effective diffusivity. However. a model with $r_0 = 300$ km, $\alpha = 250$ and time step $\Delta t = 12$ h would lead to a singular mixing event with $D_v \approx (1/\Delta t)(r_0/\alpha)^2 \approx 30$ m^2/s. Such a value is much too large compared to the real atmosphere. Even if I agree with the authors on their doubts how to interprete the observations which are, to some extent, bulk quantities, there are also some limitation on the realistic resolutions. If the typical width of the observed filament is of the order 10-50 km, this is also the order of the horizontal resolution that has to be achieved within the model. Here, again the CLaMS-mode of the ATLAS simulation is necessary. The pure ATLAS-mode is a promising approach but without applying this approach in the high-resolution mode, not useful in terms of comparison with in-situ data and of learning about the real atmospheric diffusivity. Here further discussion about the limitation of the ATLAS mode is necessary.

Minor comments:

- Title
  "transport and mixing" - in the Lagrangian picture transport means advection and mixing, so either transport or mixing would be enough
- p. 710, par 15
  "mixing ratios are conserved" - should be replaced mixing ratios are positive by design

GMDD

2, C193–C199, 2009

Interactive Comment

- p. 715, par 5
  after “The reinitialization of the parcels” include: within the boundary layers

- p. 717, par 20
  Random vertical coordinate within the layer means additional, undesired “numerical diffusivity”

- p. 718, par 5
  the 3-D triangulation for the determination of the next neighbors is certainly an improvement of the model. But it is still not clear (Fig. 2) how does this work ? First transformation of the air parcels to a unit sphere and than triangulation ? If yes, how the aspect ratio is included ? Why second neighbors ? How the second neighbors and the following merging of air parcels based on the 2-D triangulation can be understood as an approximation of the “true” 3-D neighbors. Also the impact of $\Delta z_{low/up}$ on the “true” 3-D neighbours is unclear

- p. 718, par 10-15
  It seems that the mechanism controlling the density of air parcels does work only in the 2-D approach... Why not in the 3-D approach. This part of the text is not clear

- p. 718, par 20
  The layer concept in CLaMS has two meanings: First (more important), only a layer around each air parcels is important for mixing. Second: the staggered layers are used for the determination of the next neighbors (approximation). ATLAS improves the second point but, unfortunately, not all details are sufficiently explained.

- p. 718, par 25
  “will be used eventually” - I would remove this sentence

GMDD

2, C193–C199, 2009

Interactive Comment

- p. 719, par 25
  random numbers - it seems that this effect removes the advantage of a better determination of the next neighbors
- p. 720, par 20
  the relation between the Lyapunov exponents and vertical strain is shown in Konopka et al., JGR, 2004.
- p. 721, par 5
  "If the flow exceeds a critical value λ_c...we will insert a point". This is only true if all next neighbors are separated by the same distance r. Normally, the distance to the next neighbors is around r so this condition is only statistically valid.
- p. 722, par 5
  "no constraint on the total number" - the density condition sets the limit, i.e. the mean separation is not smaller than r_0. Why Figure 16 and not Figure 4 ? Furthermore, I do not understand this Figure: I expect a minimum and not a maximum around $\lambda = 3$?
- p. 723, par 1
  "both pressure" - which both ?
- p. 723, par 10
  1-D climatology contains advective parts of transport, please mention it
- p. 726, par 5
  Eq (8) describes much more the numerical diffusion of a simple linear interpolation between 2 points separated by Δr.
- p. 729, par 5
  has has

GMDD

2, C193–C199, 2009

- p. 734, par 20
  I do not understand eq (12). One of the “model”-index should be “observ” ?
- p. 739, par 10
  the γ - remove “the”
- p. 739, par 25
  The dependence of mixing on $\lambda_c \Delta t$ was discussed in Konopka et al., 2005, Quart., J. Roy. Met. Soc.
- p. 740, par 5
  “sets in” - is becoming active
- p. 741, par 0
  due to increasing distances between air parcels which are mixed...
- Fig 2
  Please improve colors. Top right: should be mentioned that this “a view from above”
- Fig 8
  Mixing mismatch - please reformulate
- Fig 12
  check the colors
- Figures 11 and 12 are the less important figures. Perhaps you can remove them.

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