

Interactive comment on “The Lagrangian chemistry and transport model ATLAS: simulation and validation of stratospheric chemistry and ozone loss in the winter 1999/2000” by I. Wohltmann et al.

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Dear reviewer,
thank you for reviewing our paper and for your helpful comments! You might be pleased to hear that we are indeed working on a paper containing some sensitivity studies concerning denitrification and heterogeneous chemistry.

Specific comments

- Table 5: We have added a table sorted by date that shows the ER-2 flights and C424

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balloon ascents, and the inner and outer vortex flights. We did not add the measurement technique to Table 5, since the table would not be easy to read then. Since the measurement technique is briefly described in the text, we think that is a reasonable compromise.

- Page 780 lines 22–25: HCl is initialized from HALOE data. This is mentioned in line 10 in the same paragraph.
- Page 781 line 4: Thank you for pointing me to this. There was a coding error in the initialization routine for Bry. That caused some confusion in the description of the initialization in the paper. In addition, it turned out that it was not clear if short-lived substances were included or not in the used tracer-tracer relationship. I have now rephrased the paragraph to correct these issues.
 - The coding error: Bry is initialized from a tracer relationship from ER-2 data, taken from Grooß et al., 2002. Looking at Figure 3 of this paper, the tracer relationship ends at 6 ppt at a methane value of 1.64 ppm. There is no information for lower altitudes (higher methane values). Unfortunately, I did not consider the upper limit of 1.64 ppm for which the polynom fitted to the data would give valid values (as given in Table 1 of Grooß et al.). Because the polynom extrapolated smoothly to zero ppt of Bry at 1.8 ppm methane, I used the polynom up to 1.8 ppm. There are both large uncertainties in the amount of very short-lived bromine substances at the tropical tropopause and the amount transformed into product gases or inorganic bromine there, so the Bry values above 1.64 ppm methane probably still make sense. Hence, I did not change the initialization.
 - Short lived substances: The relationship does contain a contribution from the short-lived gases CH₂Br₂ and CH₂BrCl of 2–3 ppt according to the author of the data files. Since the ACATS instrument onboard the ER-2 did only measure Halon-1211, these species and all other bromine containing

species except for Halon-1211 are inferred indirectly from tracer-tracer relationships from earlier measurements.

In this regard, it is better to state that the scaling to 19.9 ppt does account for the discrepancy between the 18.4 ppt Br_y inferred from measurements of organic source gases including short-lived gases and the 19.9 ppt inferred from BrO measurements and not for the contribution of short-lived gases.

- Page 782 lines 3–12:
 - Interpolation to trajectories: The mixing ratios are interpolated from the last model output file before the measurement date. Model output is saved every 12 hours. The mixing ratios are interpolated from the irregular grid of the model air parcels to the trajectory positions by triangulation and subsequent linear interpolation from the nearest neighbors (more specifically, a barycentric interpolation in the tetrahedron of air parcels the trajectory is located in). I have added a sentence to the paragraph that model output is saved every 12 hours and slightly rephrased the description.
 - Species are initialized in four different ways in this model run:
 - a) Many species are taken from HALOE and ACE FTS satellite climatologies (in 2D as a function of pressure and equivalent latitude). I have added a note that ACE data is also a function of equivalent latitude and pressure to the paragraph.
 - b) Inside the vortex, many species are initialized as spatially constant profiles that are only a function of pressure (LACE, Mark IV). I have rephrased the paragraph to make it more clear that single constant profiles are used.
 - c) Several species are initialized from tracer-tracer relationships, with one of the tracers known from the satellite measurements. I hope this method is described sufficiently clear in the paper.

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d) All species not mentioned in the paragraph (the short-lived species) are simply set to zero. I assumed this to be implicitly clear, but have now added a note to the paragraph.

– Trajectories for the ER-2 flights are typically calculated every 10 s, but that varies with instrument and flight. The times are simply taken from the complete time series in the data files. An analogous approach is followed for the other data. Added a note to the paragraph that the trajectories are started every 10 s.

- Page 784 line 2: Replaced “sets in” by “begins”.

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