

Reviewer 2

The authors highlighted some recent changes in the FLEXPART model since the last similar publication for FLEXPART version 10.4 in 2019. The detailed descriptions of the changes are quite useful not only for the model users but also for other model developers. While the presentation is mostly clear, minor revisions are still needed. General and specific comments, as well as some editorial corrections are listed below.

We would like to express our thanks to the reviewer for dedicating time and effort to thoroughly review our manuscript and appreciate your feedback and constructive suggestions. Please see below our responses to your comments.

In the following, responses are in blue, and quoted text is show in green. Text after the little arrow '→' is newly introduced or modified manuscript text in the reaction to the reviewer's comments.

General comments:

The improved accuracy of the new version is not convincingly demonstrated from the examples in the manuscript. Although the semi-conserved property tests in section 3.2 show clear improvement of the new version, the tested properties are not exactly conserved as the authors also pointed out.

Validation of trajectories is a notoriously difficult task, since there are few (if any) data sets that provide a solid ground truth against which calculated trajectories could be compared. For the mid-to upper troposphere, where we expect the largest improvements for FLEXPART 11, this is even more the case than for the boundary layer, where at least some tracer and constant-level balloon experiments are available. Other than the dynamical tracers which we use, we are not aware of any data set that could be used for that purpose. For instance, remote sensing data of volcanic ash plumes are unsuitable because the strength, height and time variation of emissions is never known accurately enough; the vertical motions of balloons do not follow vertical air motion closely enough; on-purpose tracer releases are not available.

The tracers which we use are indeed not perfectly conserved. We agree with the reviewer insofar as this cannot be used to assess the accuracy of individual trajectories. However, we believe that our method is valid for assessing the improvement of accuracy of the model, by comparing the results before and after the changes have been implemented, and by using a large set of trajectories. It is definitely expected that a better model should lead to overall better conservation

of these tracers, since model errors will add to physical (diabatic) effects leading to non-conservation. We show an improvement in accuracy, rather than an absolute measure of accuracy.

We measure the change in properties of particles over time of two runs with identical initial conditions and meteorological input data. The only difference between the two runs is the vertical interpolation of meteorological input data. Both runs show increasing deviations of the quasi-conservative properties over time from the perspective of the initial values. As the reviewer wrote, such a deviation is not necessarily incorrect. However, we can see from the figure in section 3.2 that the largest increments in the deviations occur when in the middle between the two hours where data is interpolated from, which points towards an increased change in quasi-conservative properties due to numerical and not due to physical reasons. Although not perfect, the simulation with the new scheme results in a smaller change in tracer values over time, which, in our opinion, can only be attributed to an improvement in the numerics of the model.

The statistic results listed in Section 7 with tracer experiments show very marginal differences between the new and old versions. While Figure 6 compares the new model results with the ETEX measurements, it will be helpful to show the concentration fields predicted with the old version (or the difference between v 11 and v10.4). It will be beneficial to compare the vertical profiles of CAPTEX aircraft measurements and the predictions with both FLEXPART versions.

As mentioned before, the biggest impact of the new scheme is expected in the stratosphere, and maybe upper troposphere over mountains. It is therefore not a surprise that the comparison with ETEX does not show a substantial improvement. Section 7 primarily serves to validate that we did not break something while making all the modifications to the code. We removed statements of getting better results for FP 11 as compared to FP 10 in this section, since we agree that these are marginal. Figure 6 for v10.4 output looks close to identical to the v11 output, which we added to the caption of figure 6:

“Note that results using z coordinates and FLEXPART 10.4 do not show significant differences.”

There is no doubt that the OpenMP parallelization implementation is important for the FLEXPART users, but many details of the technical aspects are probably not needed for a scientific paper. This reviewer suggest moving some of the contents in Section 8 to a supplementary material.

We understand this argument. However, after thoughtful consideration, we prefer to keep the section within the main text as it is, because an article for GMD, as a journal specialised on describing model developments, should include the more technical model development aspects as well. We also noted that the other two reviewers did not raise this concern.

Specific:

Lines 24-25, "... they can take into account all processes occurring during transport including nonlinear atmospheric chemistry": This gives an impression that Lagrangian models can not account for such processes. However, it is not true. Although it is convenient to use the Eulerian methods for such processes, the statement could be misleading.

We corrected the statement in the following way: "The advantage of Eulerian methods is that they can take into account all processes occurring during transport including nonlinear atmospheric chemistry." → "Eulerian methods offer a convenient means of accounting for all processes that occur during transport, including nonlinear atmospheric chemistry."

Line 48, "FLEXPART combines a unique set of capabilities no other model can offer, ...": Other Lagrangian 3D particle models have most if not all the capabilities listed here. Thus it is not accurate. Please remove "no other model can offer".

We removed the statement.

Lines 149-150, "In addition, to avoid regions with low Coriolis force, we only used particles at latitudes north of 40°N and south of -40°S": Why? Can this be elaborated?

We changed the text as follows: → "We only used particles outside the subtropics and tropics, excluding the zone between 40° S and 40° N, as we expect the tracer conservation in this region to be worse in general, where the geostrophic balance is weak and deep convection is frequent."

Lines 411-412, "In fact, with the exception of FA5 and FOEX, all statistical values are slightly better for FLEXPART 11 than for FLEXPART 10": FLEXPART 11 using the z coordinate system actually has a better FA5 than FLEXPART 10.4. In addition, it is better to differentiate FLEXPART 10 and FLEXPART 10.4.

Removed the line 'In fact, ...' and changed all instances of FLEXPART 10 to FLEXPART 10.4.

Line 425-426, "We also see no systematic large differences between FLEXPART 10.4 and FLEXPART 11, except for the NMSE values which again are better for FLEXPART 11": The second part of the statement is not true.

The NMSE is lower for FP 11 as compared to FP 10, both for ETEX and CAPTEX, but we removed the sentence since the differences between all individual statistical values are not significantly different.

Line 421, "In table 1 we list the average and medians of ...": What are actually listed in Table 1?

Corrected, only means are listed.

Line 445: Please clarify what “convection computations” mean here. Does that include the horizontal transport?

We clarified this in the following way: “Convection computations” → “convection parameterisation (see section A2.1)”

Line 559, “For the largest, this ...”: What does the largest refer to?

We corrected this as follows: “For the largest, this...” → “For the largest problem size, this...”

Line 610, “part_i.nc in the output directory”: Should it be the input directory?

We moved the part_ic.nc to the options directory, since this is indeed a more logical path than the output directory.

Line 706, “..., whereas NCEP-based input comprises only pressure-level fields”: Current GFS model has a hybrid sigma-pressure vertical coordinate.

Yes, but unfortunately FLEXPART is built to ingest the NCEP pressure-level data. It would indeed be better to use the native sigma-level data. To our knowledge, nobody has adapted FLEXPART to use these data instead of the pressure level data.

Line 776, 0.002 km^{-1} : Should the unit be K km^{-1} ?

Corrected

Table A1, “E-ward & N-ward turbulent surface stress row”: The unit of turbulent surface stress should be “ $\text{N m}^{-2} \text{ s}$ ” instead of “ $\text{N m}^2 \text{ s}$ ”.

Corrected

Table A2: Please explain what α and β are.

Explanations of α and β have been added: ... and α and β are empirical expressions. → and α and β are sigmoidal functions of $\rho' = \rho/\rho_f$.

Table A3: Units are needed for some of the parameters such as $T_{1/2}$. In addition, it is better to have “1/2” as a subscript.

Thank you for pointing this out. We have added the units and written $\frac{1}{2}$ as a the subscript.

Editorial:

List of affiliations are not in order.

Corrected

Line 193: “byCassiani”-> “by Cassiani”

Corrected

Line 471,” Replace “printed” with “written” or “recorded”.

Corrected

Line 735: Remove “to” after “making use of”.

Corrected

Line 762, “turbulent modtion”: Please correct the typo.

Corrected

Table A1: What is “etadot” in the Vertical velocity unit for IFS?

Corrected to Pa/s, which is what FLEX_EXTRACT outputs after downloading the ECMWF data. See Tipka et al. (2020) for details of how vertical motion is handled.

References:

- Tipka, A., Haimberger, L., and Seibert, P.: Flex_extract v7.1.2 – a software package to retrieve and prepare ECMWF data for use in FLEXPART, Geoscientific Model Development, 13, 5277–5310, <https://doi.org/https://doi.org/10.5194/gmd-13-5277-2020>, publisher: Copernicus GmbH, 2020.