Reviewer 3

The paper is a good summary of the improvements and updates made to FLEXPART at version 11, notably use of the native eta vertical coordinates with ECMWF meteorological data, accounting for the non-sphericity of particles, improvements to the wet deposition scheme, incorporation of a linear chemistry scheme, and the use of OpenMP parallelisation. The accuracy and performance of the model is also assessed using idealised tests, historic tracer experiments and more recent real-life events. The FLEXPART community should be commended on documenting and publication of the details of their model, including keeping this current and up-to-date. I find the paper well written and thorough and have only some minor comments and suggestions detailed below. I have also included a list of typographical errors I spotted. I recommend that the manuscript is accepted for publication after these queries and requests have been addressed.

We are grateful to the reviewer, Helen Webster, for the time and effort spent on thoroughly reviewing our manuscript. We hope we have addressed your comments in a satisfactory manner and made the necessary revisions to improve the manuscript. Below, we listed 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.

1. Lines 46-48: The list of Lagrangian particle models seems to lack some of the key Lagrangian atmospheric dispersion models: MLDP0, NAME, SPRAY etc.

Our apologies for this oversight, we included NAME, SPRAY, and MLDP0:

"*Besides FLEXPART, several other LPDMs for regional and large-scale atmospheric transport modelling exist, e.g., HYSPLIT (Draxler et al., 1998), STILT (Lin et al., 2003), TRACMASS (Doos et al., 2017), MPTRAC (Hoffmann et al., 2022), and ATTILA (Brinkop et al., 2019)." → "Several other LPDMs exist, such as HYSPLIT (Draxler et al., 1998), STILT (Lin et al., 2003), TRACMASS (Doos et al., 2017), MPTRAC (Hoffmann et al., 2022), ATTILA (Brinkop et al., 2019), NAME (Jones et al., 2007), SPRAY (Tinarelli, et al., 2000) and the CMC's dispersion modelling suite (Damours et al., 2015)."*

2. Line 48 "FLEXPART combines a unique set of capabilities no other model can offer…" and line 83 "offers many features not available in other models": the authors may want to rephrase these sentences, as it could be read as though the authors are implying FLEXPART is superior to other Lagrangian dispersion models. There is much commonality amongst Lagrangian particle dispersion models and many of the capabilities listed are present in other models. In addition, some of the functionality added to FLEXPART at version 11 has been present in other models for some time. Whilst it may well be true that FLEXPART is the only model to have all of the combination of functionalities listed, other Lagrangian models have some different functionality that

FLEXPART may not (such as a Eulerian sub-grid model and radioactive decay into daughter products). The Lagrangian atmospheric dispersion modelling community benefits from different models and from the interactions within the community.

We rephrased it to:

"FLEXPART combines the following capabilities: (i) a detailed..."

3. Line 92 refers to a Gitlab repository. Has this text been updated following comments by the editor on the suitability of Gitlab?

We added the following: "Accompanying this paper is a completely revised technical documentation, including a download and installation guide, of FLEXPART (https://flexpart.img.univie.ac.at/docs); a snapshot of the code used in this work is available at https://zenodo.org/records/12706633."

4. Line 101: The horizontal spatial resolution of the ERA5 meteorological data is quite coarse compared with the resolution of the ERA5 model (~30 km). Why is this? This seems particularly relevant given the use of the native vertical coordinate system to improve particle transport accuracy in this paper. If higher resolution meteorological data is available, this will also serve to improve particle transport accuracy.

We admit that data extracted at 0.25 (or 0.28125, to be more precise) deg resolution might have lead to slightly more accurate results, but at the cost of a quadrupled volume of input data. The 0.5 resolution data set is already very large, which is the reason for the choice made. Additionally, we had the impression the that horizontal variability of meteorological parameters at the smallest resolved scales in IFS output, including ERA5, is quite damped , and thus, extracting and using the data at the highest possible resolution may not result in a lot of improvement compared to 0.5 deg.

We added the missing vertical resolution to line 101: "For the examples provided in this paper, we use the most recent re-analysis dataset of ECMWF, ERA5 (Hersbach et al. 2020), with hourly 0.5°x 0.5° data on all of the 137 model levels as input to FLEXPART."

5. Does the use of different vertical coordinate systems within and above the boundary layer (when using the eta option with ECMWF meteorological data) lead to any issues at the boundary layer top?

We have not observed any issues at the boundary layer top. There is no signal visible at the ABL line in Figure 2, but since this is an average over a large area, possible isolated issues might not show up. However, we don't expect such problems, because FLEXPART first defines whether a particle is above or within the boundary layer, with subsequent use of the eta coordinate system if within. Then, it:
1) transforms the vertical position of the particle to the meter system,
2) computes the transport, including by turbulence, within the boundary layer in the meter system,
3) transforms the particle position and vertical velocity to eta coordinates
4) performs the Petterssen correction in eta coordinates

6. Figure 1 caption “absolute latitudes of 40 and 80◦”. I was uncertain what this meant here, although it was explained in the text. Could you say perhaps ‘between 40 and 80 degrees north and between 40 and 80 degrees south’ in the caption to be clearer?

Adjusted, thank you.

7. Line 199: For readers not familiar with FLEXPART, could the options CTL and IFINE be defined?

We reworded the sentence:

“*We used short time steps LSYNCTIME=600, with both the CTL and IFINE options set to 10) to increase the accuracy of turbulent transport in the ABL.” → “We used short time steps, with the basic integration time step LSYNCTIME=600 s, and both the CTL and IFINE options set to 10 (thus allowing for reduced time steps in turbulence calculations, see section A2.2) to optimise the accuracy of the simulation of turbulent transport in the ABL.”*

8. Why is equation 5 not recovered, by setting kN and kS to be one in Equation 6? Should the two not be consistent in the limit of non-spherical → spherical?

Both equations are based on the generalized correlations for drag coefficient C_D proposed by Haider and Levenspiel, 1989:

$C_D=(24/Re)*(1+C_1ReC_2)+C_3/(1+C_4/Re)$

However, the two equations are not consistent in predicting the drag coefficients of both spherical and non-spherical particles. The fitting constants C_1, C_2, C_3 and C_4 are different in both cases. Equation 5, proposed by Clift and Gauvin, 1971, is based on empirical data of drag coefficients only for spherical particles (Figure 1 in Clift and Gauvin, 1971) and is not suitable for non-spherical particles, while Equation 6 is a semi-empirical model describing only non-spherical particles with different orientations of falling (Figure 23 in Bagheri and Bonadonna, 2016).

9. CAPTEX results: I agree that there are no substantial differences (other than the NMSE and FOEX improvements), but the language is a bit inconsistent with that used to describe the ETEX results (“slightly better”). To be consistent and objective here, “slightly worse” would be more appropriate.

This issue was also raised by reviewer #2, and we removed all mentions of ‘better’ and ‘worse’, since the differences are not significant.

10. Table A1: “used for parameterisation”. Which parameterisation?

Added specifications for each field:
Temperature → Air temperature used in convection, chemical loss, and in the calculation of relative humidity

Specific (IFS) or relative (GFS) humidity → Specific humidity used in the calculation of convection, relative humidity, and dry air density

2 m temperature → Used to calculate friction velocity, Obukhov length, and convection

2 m dew point (ECMWF only) → Used to calculate friction velocity, Obukhov length, and convection

11. Line 763: “with the value of IFINE determining the factor by which the time step is reduced”. Is this ‘further reduced’? In other words, is IFINE applied on top of CTL in the vertical?

Yes, it is. The reason is that the shortest possible basic time step in FLEXPART is 1 second. However, applying IFINE allows to even use shorter time steps than 1 second for the vertical turbulent displacements. We clarified this in the text: “...with the value of IFINE determining the factor by which the time step is further reduced.”

12. Line 772-773: What about horizontal diffusivities in the stratosphere and vertical diffusivities in the troposphere? Are these assumed to be zero?

Yes, at the moment they are assumed to be zero. This is indeed a topic where we might be able to improve FLEXPART in the future, e.g. by introducing a scheme similar to the one recently implemented in NAME (Mirza et al., 2024).
We added the following text to the paragraph in question: “Horizontal diffusion is neglected in the stratosphere, and vertical diffusion in the free troposphere. Already 20 years ago an attempt was made to include a CAT parameterisation in FLEXPART, but due to the difficulties inherent to this problem (CAT can be diagnosed only probabilistically, and it is hard to establish Lagrangian time scales for it) not pursued further. Recently work done for the NAME model (Mirza et al., 2024) may show a future way forward also for FLEXPART.”

13. Line 912; “not listed there”. It’s not clear to me where ‘there’ is.

Removed “not listed there”

14. Is the data from the simulations being made available? Please check the journal requirements.

We added all the routines and a step-by-step guide on how to recreate the input data to our submission. These can be found in the Supplement. The data set is too large (>2 TB) for direct inclusion.

Typos:

1. Line 110: “employs a hybrid pressure-base vertical coordinates” could be “employs hybrid pressure-based vertical coordinates” or “employs a hybrid pressure-based vertical coordinate system”.

Corrected

2. Line 148. I don’t think you want a ‘respectively’ here, as simulations for both heights were conducted with both vertical coordinate systems.

Corrected

3. Line 194: Space required between ‘by’ and ‘Cassiani’.

Corrected

4. Figure 3 caption “are also reported near the top” should be “are also reported near the bottom”?

Corrected

5. Line 297: “lead” should be “led”

Corrected

6. Line 328: Can you have “stronger” precipitation, or should it be “heavier”?

Corrected

7. Line 405: Should “were” be “was”?

Corrected

8. Line 408: “8 and 20 meters” – above ground level, I presume but I’d prefer this to be clearly stated.

Corrected

9. Line 412: “FA5” should be “FMS”. SCC is also slightly worse for the eta coordinate, albeit comparable for the z coordinate.

Removed this sentence, since the differences are not significant.

10. Line 475: “starting” should be “start”.

Corrected

11. The legend and caption in Figure 8 do not agree on which are the solid, dashed and dotted lines.

Corrected

12. Line 570: “That reduces” should be “This reduces”.

Corrected

13. Line 588: Remove “even”.

Corrected

14. Line 736: Remove ‘to’ - “making use of to the convection scheme” should be “making use of the convection scheme”.

Corrected

15. Line 737: Remove brackets around ‘redist’ – it is part of the sentence.

Corrected

16. Line 762: “modtion” should be “motion”

Corrected

17. Line 793: “of of” should be just “of”.

Corrected

18. Line 858: “now corresponds to a of 0.0062” should be “now corresponds to 0.0062”. Is the mention of ‘6.2’ on this line “the value of ricl,Grythe as reported in Grythe et al.”? It wasn’t clear to me.

We clarified it in the following way: “Removing the density of water from the empirical constant means that the value of $r_{icl,Grythe}$=6.2 kg/m^3, as reported in Grythe et al. (2017), now corresponds to r_{icl} = 0.0062 (dimensionless).”

19. Line 863: The use of a capital lambda for the scavenging coefficient, as opposed to a small lambda earlier could be confusing to the reader. Indeed, capital lambda is not defined.

The two different notations go back to those used in the original literature. Bulk formulations write \Lambda. We added the following clarification to the text: ‘Note that we use \Lambda here instead of \lambda to be in agreement with previous literature referring to bulk values.’

20. Line 877” “compared previous versions” should be “compared to previous versions”.

Corrected

21. Lines 889-890: “parameters pcconst, pdconst, and pnconst, respectively” would imply C, D and N (in that order), which is not the order they appear listed on line 889.

Corrected

22. Line 945: Requires an insertion of ‘iodine’ after ‘gaseous elemental’ or removal of the brackets around I2.

Corrected

23. There is some inconsistency in the formatting of units, with spaces missing between units in places (e.g., ms-1 on line 949).

Corrected and made the formatting consistent

24. Tables A3 and A4 captions refer to the species file number, which I cannot find in the tables.

Removed

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