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Interactive comment on "Development of turbulent scheme in the FLEXPART-AROME v1.2.1 Lagrangian particle dispersion model" *by* Bert Verreyken et al.

Anonymous Referee #2

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The manuscript by Verreyken and co-workers presents the development of a novel version of the widely-used Lagrangian particle dispersion model FLEXPART for the use with output from the limited area model AROME. However, the focus of the manuscript is on the development and validation of new turbulence schemes that could be used as an alternative to the default FLEXPART parameterisation that is not building on the turbulence information available from the driving meteorological model. The design and implementation of new turbulence schemes for FLEXPART certainly is an important development and may lead to improved dispersion simulations in many different areas of atmospheric transport. However, I feel that the study was not carried out with the required care and thoroughness and needs major revisions before it can be accepted

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in GMD. A detailed list of my concerns follows.

Major comments

Validation

A number of different new turbulence schemes (or various settings for these) were tested for conservation of well-mixedness and for two different case studies with surface releases. Although, the well-mixedness test is very important, it alone does not seem to be sufficient to judge which setup performance best. The surface release cases remain very qualitative in their evaluation. I had hoped for a more quantitative validation of the turbulence schemes, either by application to existing tracer release experiments or, if this is not easily possible, by an application to real-world observations made at the Maido observatory on La Reunion. The manuscript mentions observations of water vapor isotopes at the observatory, but surely there are also other observed tracers that could be used to identify the PBL influence at the site and could be compared to different transport simulations in a more quantitative way and under different mixing conditions (if possible). Such an analysis is hinted to at the end of the conclusion as part of future work, but I strongly feel that the current manuscript requires this more quantitative validation as well. Without such an analysis I don't think a clear conclusion can be drawn in terms of which turbulence scheme should be used in future applications and if the new schemes are even performing correctly at all.

Structure and Presentation

It is not always easy to follow the flow of the manuscript. It is often not well explained why and how certain things were done (see examples below). In other sections the manuscript is lacking the degree of detail that is important for a model development paper. Also, the current conclusions are lacking a clear recommendation, which of the new turbulence schemes should be used in future studies, and if the developments presented here will make it back into the main and/or WRF FLEXPART versions.

Minor comments

Abstract, last sentence: This was said before. Maybe reformulate to make it the main conclusion of the study. Also include a statement/recommendation of the default turbulence scheme to be used with FLEXPART-AROME.

Introduction: The pros and cons of Lagrangian versus Eulerian models are stated. However, this section is lacking good citations and it is also a bit too negative about Eulerian models. For example advection schemes in Eulerian models can be designed in ways that they are conserving mass and are less diffusive. But usually this comes with a prize of higher complexity and larger computational costs. But generally the statement that Eulerian models cannot do this is not valid. Also, there are other uncertainties connected to offline Lagrangian transport models. 1) temporal resolution of input meteorology, when running off-line, 2) less explicit description of turbulence (in comparison to prognostic TKE in most NWPs), exactly what the manuscript highlights later.

P2,L6ff: Regional inverse modelling studies are also an increasingly important field of application of LPDMs: eg. Stohl et al. (2009), Lin et al. (2003), Manning et al. (2003)

P2,L11f: Does this sentence still refer to different FLEXPART versions? Please mention these again with reference. Next to FLEXPART-WRF, there is also the FLEXPART-COSMO version mentioned in Pisso et al. (2019) and described in Henne et al. (2016).

P2,L15: "French metropolitan area" Does this refer to Paris or the whole mainland France domain?

P2,L20: Is AROME-SWIO also an operational model product by MeteoFrance?

P2,L24: Reference to FLEXPART-WRF publication missing. On which FLEXPART-WRF version is FLEXPART-AROME based?

P3,L9f: The sentence is incomplete. I guess it should continue after (fig 1) without starting a new sentence.

PBL diagnostics: Why is the PBL height diagnostic, which was solely based on theta_v, called robust as compared to the Richardson bulk number approach in FLEXPART? The latter is also using the theta_v profiles from AROME, but in addition it also uses wind shear information (again from AROME). Compare Stohl et al. (2005). However, FLEXPART in its original version uses an "enveloping" PBL height, which is the maximum from the neighboring grid cells and the two model time steps in memory. It also extends the PBL height in areas with large subgrid-scale orographic variability. Both approaches may NOT be justifiable for high resolution simulations and may be the reason for the "overestimation" of PBL heights by FLEXPART in mountainous terrain (P3,L11). Which approach was followed in FLEXPART-AROME? The same as in FLEXPART-ECMWF? It is also not clear how PBL heights were estimated solely based on theta_v. By a parcel method? Assuming that the PBL height is the height where theta_v is first larger than theta_v at the surface including a surplus surface temperature? Was an additional interpolation between model levels used (like in FLEXPART)?

Comparing turbulent layers and PBL heights: The TKE layer diagnosed from AROME is strictly speaking not the same as the classical PBL height. Hence, I suggest to clearly separate the naming from what is otherwise called PBL height. This is implicitly introduced in the description, but it would be better to clearly distinguish between this turbulent layer and the PBL! It would be good to clearly define this layer in section 2 and explain in more detail how it was diagnosed from the model output. Currently this is only done in the caption to Figure 2 although the resulting layer depth is already displayed in Figure 1. From this it is also clear that one cannot conclude from the comparison between turbulent layer and PHL heights that the latter is under- or overestimated (last sentence section 2). One can only say that the former is greater or smaller than the other.

P3,L15: In FLEXPART it is also possible for particles to cross from the PBL to the FT through the subgrid-scale convection scheme. Was this switched on or off for FLEXPART-AROME. The scale would probably call for switching it off but this was not clearly stated anywhere?

P3,L21: This "erratic behavior" could be avoided by detecting the layer top where at least two neighboring levels show TKE below the threshold value. From the examples given in Fig 2. It seems it is always a single level with low TKE between PBL and shallow convection zone. Does the erratic behavior actually matter for the TKE-based turbulence scheme in FLEXPART-AROME? Or is it only a diagnostic for the comparison with FLEXPART's PBL height estimation? This should be clarified in the text as well.

One last question concerning the TKE layer height: From the layer heights displayed in Fig. 1, my conclusion would be that mixing over the sea is more intensive or at least reaches higher than over the mountains. This is counter-intuitive, but possibly related to the fact that heights above ground are shown. What are the model orography heights for the 4 points for which the layer heights were evaluated in Fig 1?

P5,L15: At this point not clear what a Thomson interface is and there is no reference given either.

P5,L15 and section 3.1: How does the Thomson approach actually justify setting the density correction to zero? The density is not affected by turbulence intensity and as such density gradients are not explicitly treated by the Thomson approach.

P5,L18ff: Point out that this choice refers to the 1D, 3D options in Table 1. Please give a reference to the "diagnostic equations from Meso-NH" so that these can be found by the interested reader or even repeat them here if they are central.

P7,L3ff: The two different ways how to calculate the time step should be introduced much clearer and the terms 'bottom-up' and 'top-down' properly introduced as two ways how to calculate the turbulent time step. These terms have different meanings in different fields and in the context of the time step it remains a bit unclear why they were chosen.

Turbulent mixing length: Would it be possible to give the equations for the three different ways how L_w was calculated?

Section 4, Validation: The setup should be described with more care and detail. For example: Were mean wind fields set to zero for this case? Were actual fields from AROME used for this exercise or some standard fields? Does it matter which exact locations were chosen? The location should not matter, only the surface properties, if winds were set to zero. How many particles were used in these exercises? How many per grid column? What was the FLEXPART PBL height in these grid cells and how did the TKE profile look like. Maybe both could be added to Fig 4.

Section 4: The 3D configurations of the turbulence scheme are never discussed only introduced in section 3. Were these schemes not tested after all? If not, why introduce them in the methods sections? If they were tested, how did the results compare to the 1D cases?

P8,L26: 'TURB_OPTION=11 and 111'. In the previous sentence the settings were spelled out not just the option index given. To keep the text flowing the same should be done here. The option index could still be given in braces (wherever this helps to clarify things). The sentence is also a bit odd, because already the previous sentence said 'DEARDORFF [...] has the least accumulation', which is the same as 'best conserve well-mixed state'. Better start with 'Besides the DEARDORFF modes, modes xxxx best coserve ...'.

P8,L29ff: The discussion on L_w could be more illustrative if profiles of L_w could also be included in Fig 4 or together with PBL heights and TKE profiles in a supplement.

Figure 4/5: Why is the second WRF TKE mode called 'stable repartitioning' here? It was introduced as a 'TKE only' method above. No mention of it being stable. In the caption it should be repeated that these are results for a grid cell over the ocean.

P9,L4: I think this should be 'Near-surface concentrations".

Section 4, Fig 5: How is it possible that the vertical gradients in the simulations with new turbulence scheme are maintained over time. Even if the mixing in the shallow convection zone is smaller than in the PBL, one would expect that the vertical gradient eventually vanishes in the 24 hours of simulation, as it quickly does in the Hanna case within the PBL. In order to illustrate this more clearly, it would also be interesting to see the final mixing ratio profiles of all configurations in a comparison.

Section 5: It would be valuable if this section would show some kind of comparison with observations at Maido. Such a comparison could help supporting the authors suggestion that the new turbulence modes are superior to previous schemes. Without such a comparison there is little evidence that the performance of the new schemes is more realistic.

P10,L3: It is always confusing with LPDMs to write about ’particle transport’ which can easily be confused with aerosol particle transport. Here, it would probably work best to simply replace ’particle transport’ by ’atmospheric transport’.

Figures 6/7: Most of the text of the figure captions is also stated in the main text. Remove from caption. Rather repeat what is seen in each sub-panels. Sub-panels should also be labeled by letters.

Section 5.2: This section needs some introduction on how computation times were estimated. Were repeated runs carried out for each configuration? This is important since run-times may differ due to other processes running on the same machine and/or I/O may be influenced by other processes. It would also be helpful to mention on what architecture and with which compiler (options) and with which parallelisation approach these results were obtained. Do these timings reflect run times for the complete model runs or just for the transport part of the model? Please speculate why the increase in computation time was so much larger for the well-mixed test compared to the surface release? Why were computation times larger for the no-turbulence cases? Shouldn’t these perform much faster, since only the mean motion needs to be solved for (which was zero in the well-mixed and point release tests)? I see it is explained later on. So

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only a quick-and-dirty implementation of no turbulence was used. But then one should not compare these run-times. There is little value in it since they present some kind of artificial, never-used option.

Conclusions: These are a bit non-conclusive. So what is the recommendation for future use of the model? Which turbulence mode should be used and why?

P13,L6: Shouldn't this be 3D TKE fields? Which dimension would be dropped out for them to be 2D?

Technical comments

P2,L4: I think the sentence makes more sense if "into the atmosphere" is removed.

Figure 1: Star for mountain location almost invisible. Use different colour instead.

P3,L30: Use braces around the argument to exp.

P9,L7: 'en' should be 'and'.

P10,L4: Maido is spelled differently at different locations in the manuscript. Please unify.

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