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Geoscientific Model Development Discussions

Interactive comment on "A new Lagrangian in-time particle simulation module (Itpas v1) for atmospheric particle dispersion" *by* Matthias Faust et al.

Anonymous Referee #1

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Review "A new Lagrangian in-time particle simulation module (Itpas v1) for atmospheric particle dispersion"

Summary This paper reports on a new Lagrangian particle model (Itpas v1) that is designed to simulate atmospheric transport and dispersion processes for mineral dust released during farming activities. Itpas runs simultaneously with the numerical weather prediction model COSMO, thereby benefiting from high temporal resolution in the wind fields. Furthermore, the turbulence parameterisation of Itpas makes use of the prognostic turbulent kinetic energy (TKE) as calculated by COSMO. The model is applied to two field experiments. Measurements from these field experiments are used to con-

struct source functions of mineral dust particles resulting from farming activities (fertilizer spreading and tillage). The model simulates the transport and dispersion of these particles for several particle size classes. The results are discussed with respect to the virtual potential temperature and the TKE as predicted by COSMO.

General impression The paper is well-written and Figures are neat. While the use of the Langevin equation with the TKE to determine its parameters is not new, it is certainly good to see that more such models are being developed and coupled to different numerical weather prediction models. The discussion of the results with respect to the virtual potential temperature and the TKE as predicted by COSMO is an interesting test. However, I think the paper is too brief with respect to (i) context, (ii) model description and (iii) model validation. While the presented case study shows several interesting features, a thorough model validation is lacking.

Comments

1. Some context is missing about why the model is developed and how it will be used in the future. (i) why do the authors focus on Flexpart and Hysplit in the introduction? These models were constructed for continental transport, while from the case study I infer that problems of tens to a few hundreds of kilometers are of interest. (ii) transport and dispersion of mineral dust is mentioned as an application; could the authors provide an overview of the current state-of-the-art in that field? And how does this approach contribute in light of the current state-of-the-art? Are the results different than what one would get when using Flexpart, or a Gaussian puff model? (iii) How will the output of Itpas be used? Is a deposition map of dust particles the final goal as in Section 3? In the presented test case, one model particle represents 5 million physical particles; will that be sufficient for operational/research use of Itpas (that is, what minimum concentration levels are still relevant)?

2. Is there a particular reason for coupling Itpas to COSMO, since I understood that COSMO will be replaced by ICON in the near future?

3. While I appreciate the clear description of the model physics in Section 2.2, I think that some additional information is needed about the model: (i) Could the authors give an idea about the model's computational requirements: how long does the calculations take and on what type of machine? (ii) The paper does not mention if and what parameters need to be specified before running the model. Could the authors describe these parameters, their default value and the impact of perturbing these values?

4. Section 3.2 "Source function": I think this is an interesting approach to determine the source function. Could the authors comment on the added value of this elaborated approach (or: what would the result be if a simpler approach would be used), especially when there is long-range transport?

5. EXP1: While it makes sense from Fig 6 that the stable conditions prohibit plume rise, and consequently a lot of particles are deposited within the first kilometers, I wonder to what extend the results presented in Fig 4 are truly physical: first, if the true transport is indeed limited to only 10 km, then ltpas (driven with meteorological data with grid spacings of 2.8 km) does not seem appropriate to model this. (ii) I'm surprised that the bulk of the plume remains below 5 m: I would expect that mechanical turbulence (due to buildings, a forest) could force the plume to higher elevations. Is the effect of mechanical turbulence taken into account, and if so, how?

6. Figure 5 (a): Could the authors comment on why the horizontal dispersion depends on particle size? In particular because the spread seems symmetric around the mean path of the plume (so that a difference due to vertical wind shear can be excluded, which would show an asymmetric spread around the mean path of the plume).

7. Section 3: While the authors describe two field experiments for which they apply ltpas, no formal model validation is performed (the measurements are not used to validate the model output but to construct source function). I think the lack of such test cases is an important drawback for this study.

Minor comments

p 1, line 6: "approximation": I would suggest to be more specific since all models use approximations at some point

p 2, line 9: “uncertainties due to turbulence” → I suggest “deviations due to turbulence”

p 2, line 20: what is the time step of ltpas? Since it uses NWP data with higher resolution than considered in Seibert (1993), the time step should be much smaller than a few minutes?

p 2, line 24: I suggest to add some motivation for avoiding temporal interpolation

p 3, line 19: “There is only a weak link between ltpas and COSMO.” Could ltpas be used with data from other NWP models?

p 3, line 27: why is the forward Euler method used? It it considered sufficiently accurate because the turbulent velocity is expected to fluctuate around 0?

p 3, line 28: “Since the particle is not allowed to leave the boundary layer directly, the model checks if the particle is still inside the boundary layer after the motion.”: (i) how is the boundary layer height determined? (ii) In contrast, Verreyken et al (2019) use the TKE to allow "novel turbulent modes [...] to mix boundary layer air with free-tropospheric air masses". (iii) Particles can only leave the boundary layer via the resolved mean wind?

Verreyken, B., Brioude, J., & Evan, S. (2019). Development of turbulent scheme in the FLEXPART-AROME v1.2.1 Lagrangian particle dispersion model. Geoscientific Model Development, 12(10), 4245-4259.

Figure 1: There should be an option "No" starting from the question "at surface?" that leads to "particle alive".

p 4, line 1: what is the motivation for the reduced approach? I can think of a reduction in calculation time, but that might not matter too match if only few particles move above the boundary layer.

p 5, line 23: The Lagrangian time scale tau_L is a vector (dependent on the spatial direction), so that the expression dt » tau_L is incorrect. I assume it should be valid for each spatial direction, so that dt » tau_L_i with i ={x,y,z}.

p 5, Eqs (3) and (4): some additional information or a reference would be welcome - why is it defined the way it is and what are the underlying assumptions and implications?

p 5, line 26: do the authors implicitly assume Gaussian turbulence?

p 6, line 9: "t" is not defined here (unless "dt" was meant)

p 6, Eq (9): "sigma_u" should be "sigma" (omit the subscript)

p 7: Eq(13): brackets are missing after "exp"

p 8, line 5: I suggest to replace "vertically" by "perpendicular"

p 9, line 10: "conservative": while this is conservative with respect to the released number of particles, it is not conservative with respect to the impact (underestimating the source = underestimating the impact)

p 13, Figure 6: the mean trajectory and the standard deviation suggest that the bulk of the plume is lifted from the ground. I would expect instead that the plume is mixed homogeneously between the surface and the top of the plume (which is also what Figure 5, c, suggests).

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