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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.

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1 Review #1

We would like to thank the Editor and the reviewer for their time spent on the manuscript and the comments and suggestions made. We carefully considered all of them; they helped us to improve the manuscript. Please find below the point-by-point reply with reviewer's comments printed in italics. Authors' comments are given below the reviewer's comment.

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 construct 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.

Many thanks for this encouraging comment. We have taken on your comment regarding the degree of detail of the manuscript's content and extended the corresponding paragraphs regarding context, model description and model validation. Please see below for further details on changes made.

1.1 General 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)?

Many thanks for this detailed comment, which we would like to address following the structure of your comment. (i) Our intention behind starting the introduction section with FLEXPART and HYSPLIT is that readers may not be familiar with the general concept of a Lagrangian particle dispersion model, however, FLEXPART and HYSPLIT are well-known and widely applied models in the broader atmospheric research community. By referring to a generally known model system, we aim at providing the reader with a rough idea on the direction the manuscript is heading thematically before we get more specific on the explicit outcome of the presented work.

(ii) Thanks for pointing this out to us. For a better understanding of Itpas' applicability, we have added a section presenting a brief overview on dust modelling in general and associated challenges to the work presented in order to provide a broader context for this study. FLEXPART is designed for global and mesoscale applications. For applications at smaller scales, there are models like microSPRAY for local-scale phenomena

such as dispersion in street canyons; these models are often driven by LES data. With Itpas we are somewhere in between the mesoscale and local-scale application. We designed our model for particle transport ranges that are too long to be captured by the (local) micro-scale models, but at the same time for particle sources that will likely be underrepresented in mesoscale model settings.

(iii) Generally, there are several options to use the Itpas model output. In order to illustrate the range of possibilities, we would like to first lay out how we use the model output in our research. In the framework of the research study, Itpas was developed, we focus on the vertical spreading of the trajectories. This allows for retrieving information on how well the model performs regarding mixing particles vertically over the depth of the boundary layer. This is a key performance measure for this kind of model. As the model outputs the trajectory data for every individual particle, various model applications are reasonable as different kind of parameters can be retrieved. For a study focusing on aerosol particles, the entire path from source to sink may be of interest. For studies of air quality, the trajectory density might be considered in more detail. And for studies of the airflow, the particle trajectory itself may provide the most relevant information. Ultimately, the aim of this study is to illustrate possibilities using the trajectory data creatively - by itself and in combination with other atmospheric data. All post-process examples are freely available on GitHub.

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?

There is no particular reason in the sense that Itpas can only be coupled to COSMO. Despite the ICON development and COSMO's retirement as an operational weather forecast model, COSMO still serves as a state of the science atmospheric research model which is used by a broad scientific community.

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?

Many thanks for your question. Regarding (i), the calculation time depends on the number of particles and how long they remain in the atmosphere. But also on how strong the particles are dispersed in the model domain. We did not perform specific experiments on the calculation time; we run our simulations on different servers with 36 processors. The actual calculation time depends on the processor generation, which was different for the different servers. However, we found that the simulation of EXP2 with 270k particles roughly takes 10 times longer than the simulation without particles. On our most modern machine (Intel(R) Xeon(R) Platinum 8160 CPU; 2.10GHz) that were 25 minutes for the experiment without and 260 minutes for the experiments with the particles. The simulation of EXP1, where most particles fall down directly, took only 40% longer than the no particle case.

(ii) A description of how to set up the model is included in the README-file of the model that we now added to the supplement.

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?

With the for this application developed source term, we aim at representing the initial

dust plume emitted by the tractor's tool as accurate as possible. The benefit of this method becomes more visible when discussing possible simplifications. The most simple approach would be to use two point sources (one for each measurement height) and use the observed particle number as input. Hereby, we would miss the particles underneath, between and above the inlets of the measurement device. This points towards the necessity of a vertical profile. But by only considering one profile we do not fully represent the particle number of the entire plume. Consequently, we need to define the volume of the particle plume. This brought us to our 3D bubble approach as presented here.

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 Itpas (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?

Many thanks for pointing this out. With regard to the first part of your comment (i), indeed, the horizontal resolution is not sufficient for such a short transport range. We also did not expect this result beforehand and we would like to explain how we think the results shall be understood. EXP1 should be considered as no transport case because the particles fall down directly after emission and the only precondition that allows for the calculated transport is the fact that small particles have small settling velocities.

(ii) The answer to this question has two aspects to consider. First, the model does not take into account small surface structures like trees, buildings or forests that could force a vertical movement of the plume. If the dust plume would pass a forest or an urban area it may slow down because of a reduced wind velocity in the COSMO model. But the particles would pass the area without being captured or lifted. Nevertheless, mechanical lifting is included in the model to account for changes in orography. However, this effect is not evident from our figures because there the relative height above the surface is shown.

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).

Of course. This effect comes from the fact that there are way more small particles in the simulation than larger ones. With increasing particle number, the chances for outliers increase.

7. Section 3: While the authors describe two field experiments for which they apply Itpas, 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.

The manuscript aims at addressing two aspects of aerosol dispersion modelling, here discussed for dust particle emission from arable land driven by mechanical soil preparation: (1) The presentation of a dust emission function that reflects the artificial (mechanically driven) nature of the dust entrainment process - other than aeolian, wind-driven emission for which the emission is a function of the wind speed. (2) The representation of the dust particles trajectory through the atmosphere. For the latter motivation, in particular, the model's ability to reflect the turbulent nature of the boundary layer

off-setting the mean travel path of an airborne particle is focused. Other than for wind-driven soil erosion, where emission fluxes are calculated as a function of wind speed, mechanically driven dust entrainment has up to our knowledge not been parameterised explicitly so far. As vital to the accurate representation of particle trajectories, we determine a source function from particle measurements obtained during the entrainment process (bypassing tractor pulling a tool disturbing the soil). Used as input information determining the particle source function, these data cannot be used for validation anymore. As an accurate as possible source function is essential to the calculation of the aerosol dispersion, and the measurements at source were not suitable for validating the transport anyway due to its too short distance, we decided to use the measurement data to obtain the best estimate of the particle entrainment. As said above, getting the source term right is essential to the correct representation of the particles' trajectories. This is followed by an as accurate as possible representation of the atmospheric dynamics, which ultimately determine the trajectories' pathway. To validate this thoroughly, a specific to this needs designed measurement setup would be desirable. In particular, having particle sampler at different height and different distances from the source in order to estimate concentration gradients and transport altitudes. As these data are currently not available, we wish to get the opportunity to thoroughly validate the here presented model system in future. Comparing against satellite retrieved aerosol concentrations fails due to too low aerosol concentrations. The second focus of our study is on evaluating the dynamics of the ABL, in particular the impact of its diurnal cycle on dust aerosol dispersion. The NWP model COSMO is well established and thus very likely able to represent correctly the atmospheric dynamics. Our particle trajectory model bases on well-known approaches too: we use the Petterson scheme for online trajectory calculation (Miltenberger et al. 2013) and the turbulent fluctuations for the LPDM (Hall 1975). In concert, known and established model components are used in our approach. The novelty we added to this model-setting is the use of the high-frequency TKE information to trigger the turbulent fluctuations on the mean wind component. Having the "ingredients" to an accurate trajectory calculation in mind, the best chance to evaluate particle motion is the behaviour of the particles in the mixed ABL. Up to now, and based on our results, we can say that the particles do what we would expect from the theory. In a nutshell: The particles are well mixed over the depth of the boundary layer, we do not have accumulations at the surface or at the ABL's top, and we have no overshooting above the ABL and no drastic loss at the surface.

1.2 Minor comments

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

We appreciate the reviewers suggestion and understand its argumentation, however, we nevertheless prefer to use the term approximation here to specifically underline that the widely common approach is to bypass an explicit parameterisation.

p 2, line 9: "uncertainties due to turbulence" > I suggest "deviations due to turbulence"

Done

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

The Itpas time step is the time step of the forecast simulation. We recommend using Itpas for simulations with a high spatial resolution (below 0.1°). For such simulations, the time step is, in general, less than 60 seconds.

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

On page 2 line 23 we state "This is a crucial issue, especially for small-scale applications at short time scales."

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

Yes, this is one big advantage of the "weak link" between Ipas and COSMO. Itpas could also be coupled to other NWP models because it has its own I/O system and 'only' need the data stream of the wind, turbulence and a view other variables and a call statement each model time step. Currently, the structure of Itpas matches with the structure of COSMO though.

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

For NWP models, the turbulent wind is completely random. Thus, calculating the new position directly or via iteration provides similar results. In essence, the turbulent wind component remains a random jump in a random direction. Additionally, the turbulent part of the motion is for most cases significantly smaller than the mean part of the motion. So the possible error of the simple integration is comparably low. For the mean wind motion, we use an accurate integration scheme.

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 freetropospheric 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.

(i) We use the boundary layer height that is provided by COSMO. In COSMO, the boundary layer height is determined with the bulk Richardson method, which describes the depth of the boundary layer as the height where the bulk Richardson number reaches a critical value, which is set to 0.33 for stable and 0.22 for unstable conditions.

(ii) Many thanks for pointing us towards this work. We absolutely agree, turbulent mixing at the upper edge of the boundary layer and thus entrainment of air into the free troposphere is an interesting question, which we will consider for future development.

(iii) In the current model version, particles are somewhat trapped in the boundary layer. Also, particles that were lifted by the mean wind through the boundary layer's top will be reflected at the layer's top. However, particles can leave the boundary layer via orographically lifting or when the ABL collapses (e.g. after sunset) around the particles. In the latter case, the particles are then situated within the residual layer above the top of the newly forming nocturnal boundary layer.

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

Yes, thanks, changed.

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.

During the night time, most of the particles are above the shallow nocturnal boundary layer within the residual layer. During these hours, the calculation can be faster.

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

Done

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?

The reference for this is Hall (1975) which is already included. Indeed, it is not obvious for the reader that this reference corresponds to the equations (2 - 4). This will be clarified.

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

In the LPDM, the turbulent fluctuation is defined as:

$$\vec{u}'_{t+1} = \vec{a}\,\vec{u}'_t + \vec{b}\,\vec{\xi}$$

where the first term includes the current direction of the turbulence and the second term adds random noise to the system. Since the random number $\vec{\xi}$ is taken from a Gaussian distribution the turbulent fluctuation appears in this shape as well.

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

Yes, t was meant, done

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

Done

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

Done

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

Done

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)

We agree, underestimating the strength of an aerosol source may ultimately result in

an underestimation of the aerosol impact. In this case here, we are confident with our approach as these particles close to the surface may deposit rather sooner than later.

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).

Around noon and during the early afternoon, dust is mixed homogeneously over the depth of the boundary layer due to convective mixing. In the evening after sunset, the plume appears lifted above the ground as described in the manuscript. However, the illustration of the mean trajectory has the weakness as it is defined as the mean of the trajectories that reach the eastern edge of the domain. As a consequence of this definition, particles that tend to travel on lower altitude, and may also deposit earlier, are excluded. Thus the mean trajectory with its standard deviations may appear located at higher altitudes.

References

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