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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 #3

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.

The objectives of this paper are to present and to exemplify a new Lagrangian Particle Dispersion Model (LPDM) called "Itpas". As the other models in this category, Itpas computes multiple individual trajectories of air parcels (possibly carrying pollutants). The air parcels are transported by the mean components of the wind velocity and dispersed by the fluctuating components of the wind velocity. The velocity fluctuations are due to the turbulence and represented as random deviations from mean trajectories. The fluctuating components of the wind verify the Langevin equation and are modelled according to Thomson proposals.

The parameters of the LPDM are the standard deviations of the wind velocity components and the Lagrangian time scales, which can be related to the Turbulent Kinetic Energy (TKE) of the flow. As argued by the authors, the distinctiveness of Itpas is to use the high-frequent wind information and the prognostically calculated TKE issued by the German Weather Service's mesoscale weather forecast model COSMO. Moreover, Itpas is coupled on-line with COSMO. The authors give an example of application of the COSMO-Itpas modelling chain for a case-study of agricultural solid particle emission in Eastern Germany. The simulation results regarding horizontal and vertical transport and dispersion of the particles are discussed with regards to the circadian evolution of the turbulent Atmospheric Boundary Layer (ABL). As underlined by the authors, the results suggest that the Itpas model represent correctly and quite accurately the transport and dispersion of the emitted agricultural particles. The paper is well-written and well-structured. It is interesting and worth being published. I have some remarks and questions for the authors, which should be answered before the publication of the paper.

Many thanks for your encouraging comment. We have carefully considered your comments made below and provided answers to your questions.

1.1 General comments

Page 3 - Line 9 - Is it possible to use Itpas both on-line and off-line using either COSMO weather forecasts or COSMO weather analyses? Can the authors comment on the applicability of these two approaches?

Currently, the model runs as on-line application only. In an off-line setting, one crucial issue arising is the interpolation in time between the available input data. Depending on the input model this time increment can be up to six hours, depending on the data set used (e.g. some reanalysis data are available at 6-hourly resolution). But this is critical for applications with a time scale of only a view hours. In our research framework, we aim at model-based studies at a regional scale in space (a few hundreds of kilometres) and short temporal scale. In such a setup the simulation benefits from the online system because the temporal interpolation and the associated error can be avoided.

Page 5 - Line 27 - I wonder if COSMO can provide only the TKE (and horizontal and vertical diffusion coefficients) or if the meteorological model could issue the standard deviations of the three velocity components? For the LPDM, the anisotropic fluctuating components of the velocity would be much more interesting than the TKE.

Since we are calculating a particle motion for every time step of the NWP model, anisotropic fluctuations are included in our particle motion. The TKE induced turbulence is put on top to create the particle dispersion.

Page 6 - Line 3 - The "m_i" factors describe the weighting of the TKE in the three spatial directions. The values of these factors depend on the stratification conditions in

the ABL. Could the authors explain in more details how the "m_i" factors are related to the components of the mean wind?

Page 15 - Line 12 - Most of LPDM dedicated to local or regional scale simulations use the TKE to evaluate the variances of the velocity fluctuations and the Lagrangian time scales in the three spatial directions. This is probably less the case of LPDM adapted to larger scales like FLEXPART or HYSPLIT. The difficult point with TKE remains to distribute the turbulence between the space directions. Could be the authors recall how they proceed in Itpas (see my previous question about Page 6 - Line 3) and comment on this aspect?

We as the two comments above refer to the same topic, we chose to address them at once. We thank you to pointing this out. Indeed, the distribution of the TKE is an important attribute of the model and we have addressed briefly only. We provide more details on this in the revised version of the manuscript.

We distribute the TKE with the fractions of the mean wind, whereby the mean wind in the model fluctuates with every time step. So, in stable conditions for which the TKE is low, the vertical turbulent fluctuation is suppressed. In unstable conditions when the TKE and the mean vertical wind increases, we see stronger vertical turbulent fluctuations. The combination of the fluctuating mean wind and the vertical turbulence then produces the vertical mixing that we can observe for EXP2. For a better understanding of the interaction between mean and turbulent wind components, we added an additional figure (Fig. 7) to our discussion.

Page 6 - Line 16 - I don't see any major difference between the Itpas model and the FLEXPART or HYSPLIT models. Could the authors comment on discrepancies, if any, between Itpas and these models?

The main difference to FLEXPART and HYSPLIT is, that we use the prognostic TKE from the driving NWP model for our calculations. Thus, we see our model being applicable to smaller-scaled processes.

Page 9 - Line 6 - I would not say that the flow conditions above the ABL are nearly laminar. The authors should consider revising this sentence.

From a synoptic point of few, we would describe the atmosphere inside the ABL as turbulent and above as non-turbulent. But indeed the sentence as it was written is a simplification. We have clarified the wording.

Page 9 - Figure 3 - I wonder if the source term modelling depicted in Figure 3 applies for both EXP1 and EXP2. This is not clearly mentioned in the paper. Can the authors clarify this point?

For EXP1 and EXP2 individual source terms were obtained based on the corresponding measurements and used, whereby Fig. 3 only shows an example of the procedure.

Page 9 - Line 19 - The number of numerical particles (100,000 in EXP1 and 270,000 in EXP2) used in the Itpas simulations seems to me quite low. I wonder if this number is enough at least in EXP2 with particles supposed to travel several hundreds of kilometers. Was a sensitivity study about the number of numerical particles carried out by the authors?

There are no particle sinks in the model beside of the surface and the domain edges. Especially for the uplifting case, we do not have big losses once the particles start

to rise. We checked for the minimum necessary particle number and above 50k particles we do not see qualitative differences in the results. This means with at least 50 thousand particles we were able to produce similar horizontal trajectory patterns and vertical mixing like with 500 thousand or one million particles. Of course, a larger sample provides a more robust statistic but it also yields to higher computational costs. With a particle number with an order of magnitude of 10^5, we found a good balance for the presented simulations.

Page 10 - Line 5 - The source term in EXP1 and EXP2 is contained in a volume of about 10x10x5 m3. The initial distribution of the numerical particles in this volume is given by a detailed model. Is it really necessary to be so precise (see Figure 3) when considering the horizontal and vertical dimensions of the simulation domain for the atmospheric transport and dispersion?

We need to define bubble-shaped volume calculate the expected number of mobilised particles from the measurement points. Inside the volume especially the vertical distribution is significant. The closer the particle starts to the surface the lower is there chance to get into the uplifting motion. The horizontal distribution inside the start volume is not as important as the vertical.

Page 11 - Figure 4 - In EXP1, it is not clear for me if the particles are more or less lifted depending on their diameters. Can the authors clarify this point?

Yes, in essence. During EXP1 the atmospheric conditions were such that the upward motion was low and lifting forces counteracting gravitational settling were minor. So the altitude the particles have shown in Fig. 4 is basically the height up to which the tractor's tool mechanically entrains the particles. In its model representation, the height above ground particles can reach as a function of the particle size ultimately depends on the measured vertical profile for the different size classes. For your information, vertical profiles and concentration arrays for all size bins are included in the new supplement (Fig. S1 - Fig. S4)

Page 11 - Figure 4 - Moreover, I'm concerned how the meteorological model can give information so close to the ground and along a so short horizontal distance (10 to 20 km) and height (5 m). As for me, there is an inconsistency between the space and time resolution of COSMO meso-scale weather forecast and the micro-scale transport and dispersion of the particles in EXP1. Explanations and justification from the authors are needed here! (I'm more confident with EXP2 simulation.)

Thank you for bringing up this. We are agree that there is a conflict in the spatial resolution. In the transport range of this simulation there are other requirements for the model that COSMO cannot necessarily fulfill. This includes e.g. structures like buildings and forests that feedback on the wind. We have added a paragraph on the limitations. EXP1 should be considered as a case without transport. The particles were lifted mechanically and deposit again right after. Since it takes some time for the particles to settle down they get transported by the horizontal wind, but this transport is not reliable as described above.

Page 12 - Figure 5 - I'm a bit surprised by the large horizontal expansion of the particles plume in Figure 5a even if explanations are given by the authors in the paper (development of the ABL and turbulent diffusion around noon - see Page 14 - Line 9). I'm even more surprised by the vertical ascending motion not of the smallest particles (less than 1 or 2 μm), but of the largest particles (up to 30 μm). Looking at Figure 5c, it seems that there are only very few differences between the aerodynamic behaviour of the smallest and largest solid particles. Can the authors comment on this point?

The horizontal spread depends on numerous atmospheric conditions like discussed in the paper. In other test cases during the model development, we also saw more compact plumes. Also, vertical mixing is a decisive point for the horizontal dispersion. In situations with strong vertical mixing, like during our EXP2, vertical shear of wind speed and direction generally fosters horizontal dispersion.

In our understanding the even mixing of all particle sizes is plausible. As smaller particles have a smaller particle mass (assuming similar density), larger particles show higher settling velocities. The settling velocity for a particle with a diameter of 30μm is around 7.5 $cm\,s^{-1}$ and when the vertical wind velocity (mean wind + turbulent wind) has a higher value then the particle will rise (in the model's world). Vertical wind velocity in this order of magnitude is not unusual for a convective boundary layer like in our test case.

Page 12 - Figure 6 - This is not easy at all to figure out the gradient of the virtual potential temperature just by looking at Figure 6. It would be simpler to determine the stratification of the ABL by visualizing vertical profiles of the temprature gradient graphed at successive hours of the day. I suggest the authors to add this information in supplementary materials.

We agree and added a corresponding figure to the appendix (new Fig. A1)

Page 14 - Line 4 - What is supposed to be evident is actually not so obvious. See my remark just before.

It shall become evident that the boundary layer becomes unstable. However, we agree that the sentence is ambiguous and we have clarified the wording.

Page 14 - Line 19 - What are the computational times to simulate EXP1 and EXP2? Would it be possible to use Itpas off-line? What would be the difference in the computational times?

Itpas is designed as an on-line application. In EXP1 where (nearly) all particle deposit within the first minutes the running time is comparable to a simulation without particles. EXP2 took roughly ten times longer than the simulation without particles. Our simulations of EXP2 on 36 processors (Intel(R) Xeon(R) Platinum 8160 CPU; 2.10GHz) took 260 minutes compared to 25 minutes without particles. But just for curiosity: If we could have the same data available as in the on-line coupling for an off-line run, we would expect that the simulation would take around 235 minutes on a serial process on the same server because of the insufficient parallelisation. Please note, that we added a new section about the model performance to the manuscript.

Page 15 - Line 12 - Most of LPDM dedicated to local or regional scale simulations use the TKE to evaluate the variances of the velocity fluctuations and the Lagrangian time scales in the three spatial directions. This is probably less the case of LPDM adapted to larger scales like FLEXPART or HYSPLIT. The difficult point with TKE remains to distribute the turbulence between the space directions. Could be the authors recall how they proceed in Itpas (see my previous question about Page 6 - Line 3) and comment on this aspect?

Please see above for an answer to this question.

Page 15 - Line 16 - According to the authors, the area affected by agricultural emissions are "several times larger" than by wind erosion. This is not obvious. I

wonder why?

Wind erosion can only take place in agriculture when sufficient wind and non-vegetated fields occur together on sandy soils. This can happen for a time period in spring and late summer/autumn. On the other hand, dust emission can also occur during agriculture-related activities, e.g. ploughing, spreading of fertiliser, harvesting or simply driving over the field with heavy machines. Then the emission does not depend on the wind. Depending on the atmospheric situation, this may mean that dust is only whirled up (EXP1) or that dust becomes airborne and gets transported away (EXP2).

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