

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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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.

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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.

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?

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.

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?

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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?

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.

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?

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?

Page 10 - Line 5 - The source term in EXP1 and EXP2 is contained in a volume of about $10 \times 10 \times 5$ 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?

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?

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.)

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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 behavior of the smallest and largest solid particles. Can the authors comment on this point?

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 temperature gradient graphed at successive hours of the day. I suggest the authors to add this information in supplementary materials.

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

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?

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?

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?

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