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Education and research: Initial development of the Atmospheric Lagrangian Particle Stochastic (ALPS) Dispersion Model

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The Atmospheric Lagrangian Particle Stochastic (ALPS) dispersion model was created as an experimental student project and tested under idealized and complex atmospheric and topographic conditions. The challenge of the project was to bring current scientific technology to the direct involvement of students in the framework of problem based learning educational theory. The model simulates dispersion of a passive scalar in the atmosphere by calculating a large number of Lagrangian particle trajectories. It uses meteorological model output to obtain mean meteorological fields. The predicted turbulence kinetic energy (TKE) from a higher order turbulence closure nonhydrostatic meteorological model is used for the simulations. Idealized tests showed that ALPS is correctly responding to different static stability conditions and associating dispersion of particles according to the magnitude of turbulence, satisfying the well-mixed criterion.

Keywords: student project, air quality modelling, idealized simulations

1. Introduction

Air quality models are used to simulate and predict the concentration of a passive scalar (a pollutant) in the atmosphere. They are used in theoretical studies, in determining present source-receptor relations, or to forecast the dispersion of a pollutant in case of hazardous accidental release. Air quality modelling is applied to a wide range of domains, from short-range transport inside of a building, up to long-range transports of pollutants across several thousands of kilometers.

There are several basic types of deterministic numerical air quality models (Collett and Oduyemi, 1997). Box models calculate the concentration of a pollutant within a rectangular box, assuming homogeneous conditions and using mass balance equation within the box. Gaussian models are widely used. They are based on the assumption that dispersion of a pollutant can be described by a modified Gaussian or normal distribution. Although easy to use with easily measurable meteorological parameters, their disadvantages are assumptions of homogeneous and stationary meteorological conditions, relatively flat topography and inability to work in calm conditions. Eulerian models solve the conservation of mass equation for a given pollutant in an Eulerian framework of an equidistant grid. Giving good concentration information through domain, they are computationally expensive and have a problem of closure methods for resolving the eddy diffusivity term in model equation. Lagrangian models have the reference system following the prevailing vector of atmospheric motion. Lagrangian box model is similar to the Eulerian box model, with the difference that in Lagrangian box model the box is advected horizontally with the mean flow. Lagrangian particle models are the most recent and powerful computational tool for numerical discretization of a physical system, successful in applications that range from atomic scale (electron flow) to astronomical scale (galaxy dynamics) (Zannetti, 1990). Pollution source quantities are represented by a finite number of infinitesimal particles through small emission time intervals. Dispersion of a pollutant is numerically simulated by calculating Lagrangian trajectories of great number of these particles. Each particle moves due to mean fluid velocity and due to turbulent subgrid-scale velocity. Turbulent velocities can be calculated deterministically or stochastically. Stochastic approach is based on Langevin equation. The use of this approach in air quality modelling is growing rapidly in the world. For example, UK Meteorological Office model NAME was applied to various problems such as long range transport of radio-nuclides, production of ozone or dispersion at small scales near buildings (Middleton, 2002). Becker et al. (2002) have used the LaMM5 (a system of online-coupled meteorological model MM5 and Lagrangian particle transport model) to calculate 4D source attribution for the area of Berlin. Carvalho et al (2002) have studied the dispersion of pollutants released from tall and low sources using Lagrangian particle model LAMBDA. Koračin et al. (1998, 1999) have applied Lagrangian particle dispersion model LAP using Mesoscale Model 5 (MM5) (Grell et al., 1995) as meteorological input to transport and dispersion of chemical tracers in complex terrain.

Previous experiences and dispersion model applications in Croatia were based on the Gaussian plume model which is commonly used (Šinik, 1981; Vidič, 1981, 1989; Šinik et al., 1984), and Lagrangian box model which has been used in several studies of long-range transport of sulphur (Klaić, 1990; 1996; 2003).

The first version of Atmospheric Lagrangian Particle Stochastic (ALPS) model was created as an exercise during a graduate course »Atmospheric

Modelling« at the Department of Geophysics of the Faculty of Science, University of Zagreb, under the guidance of Prof. D. Koračin. It is a Lagrangian random particle model that is based on statistical approach by modelling the randomness of the trajectories of fluid elements. The aim of this project was to introduce students to the problem of numerical modelling by combining education and research. ALPS was created using a basic algorithm of Langevin equation models as presented in Koračin et al. (1998, 1999). The challenge was in finding solutions for using available meteorological model data, choosing turbulence representation, dealing with interpolation within the grid, reflection at the boundaries, etc.

The aim of this paper is to present ALPS model, its characteristics and results achieved in this phase of development, as well as new directions and possible applications to air quality modelling studies.

2. ALPS Model

In Lagrangian particle motion turbulent diffusion is found to be similar to Brownian motion and can be represented by Langevin stochastic differential equation:

$$\frac{du}{dt} = -a_1 u + b\xi(t) \tag{1}$$

where u is particle velocity, t is time, term $-a_1 u$ represents viscous drag, and term $b\xi(t)$ represents rapidly varying acceleration component. Particle trajectories are calculated integrating these stochastic incremental changes in Lagrangian velocity. For detailed review of Langevin equation and the rest of physical and mathematical foundations of stochastic Lagrangian models of turbulent diffusion see Rodean (1996). The basic concepts of Lagrangian particle models can be found in Zannetti (1990).

In ALPS, particle position (x, y, z) at every timestep is calculated by:

$$\begin{aligned} x(t+\Delta t) &= x(t) + (u(t) + u_r(t)) \cdot \Delta t \\ y(t+\Delta t) &= y(t) + (v(t) + v_r(t)) \cdot \Delta t \\ z(t+\Delta t) &= z(t) + (w(t) + w_r(t)) \cdot \Delta t \end{aligned} \tag{2}$$

where u, v, w are components of mean wind velocity (from meteorological model), and u_r, v_r, w_r are subgrid-scale velocity components representing turbulent diffusion. Subgrid-scale velocity components are determined as:

$$\begin{aligned} u_r(t) &= u_r(t-\Delta t)R_u(\Delta t) + u_s(t-\Delta t) \\ v_r(t) &= v_r(t-\Delta t)R_v(\Delta t) + v_s(t-\Delta t) \\ w_r(t) &= w_r(t-\Delta t)R_w(\Delta t) + w_s(t-\Delta t) \end{aligned} \tag{3}$$

where R_u, R_v, R_w are the Lagrangian autocorrelation functions, and u_s, v_s, w_s are random velocity components. These random components are determined from Gaussian probability distribution with zero mean and standard deviation σ_{us}, σ_{vs}, σ_{ws} respectively. Taking variances of (3) we can see that:

$$\begin{aligned} \sigma_{us}{}^2 &= \sigma_{ur}{}^2 \left(1 - R_u{}^2 (\Delta t)\right) \\ \sigma_{vs}{}^2 &= \sigma_{vr}{}^2 \left(1 - R_v{}^2 (\Delta t)\right) \\ \sigma_{ws}{}^2 &= \sigma_{wr}{}^2 \left(1 - R_w{}^2 (\Delta t)\right) \end{aligned} \tag{4}$$

where σ_{ur}, σ_{vr}, σ_{wr} are standard deviations of u_r, v_r, w_r, and represent turbulent fluxes $\overline{(u'u')}$,$\overline{(v'v')}$,$\overline{(w'w')}$, at the particle location:

$$\begin{aligned} \sigma_{ur}{}^2 &= \overline{(u'u')} \\ \sigma_{vr}{}^2 &= \overline{(v'v')} \\ \sigma_{wr}{}^2 &= \overline{(w'w')} \end{aligned} \tag{5}$$

The autocorrelation functions are related to Lagrangian time scales T_{Lu}, T_{Lv}, T_{Lw}:

$$\begin{aligned} R_u (\Delta t) &= \exp(-\Delta t \,/\, T_{Lu}) \\ R_v (\Delta t) &= \exp(-\Delta t \,/\, T_{Lv}) \\ R_w (\Delta t) &= \exp(-\Delta t \,/\, T_{Lw}) \end{aligned} \tag{6}$$

Lagrangian timescale represents the time over which the velocity of a particle is self-correlated or roughly the time over which a particle maintains its initial velocity before experiencing a turbulent collision (Daoud et al., 2003). Since Lagrangian timescales are very complicated to measure, efforts have been made to find the relation between Lagrangian and Eulerian frames of reference for measuring turbulence. Using experiments in which both Lagrangian and Eulerian turbulence was measured, Hanna (1981) and Hanna et al. (1982) developed a set of parameterizations for T_L in case of different stability regimes. ALPS uses a combination of parameterizations similar to those from Zannetti (1990).

In unstable conditions:

$$\begin{aligned} T_{Lu} &= 0.17 \frac{z_i}{\sqrt{\overline{(u'u')}_m}} \\ T_{Lv} &= 0.17 \frac{z_i}{\sqrt{\overline{(v'v')}_m}} \\ T_{Lw} &= 0.17 \frac{z_i}{\sqrt{\overline{(w'w')}_m}} \end{aligned} \tag{7}$$

where z_i is the depth of the mixed layer and $\overline{(u'u')}_m, \overline{(v'v')}_m, \overline{(w'w')}_m$ are the maximum variances in the domain.

In stable conditions:

$$
\begin{aligned}
T_{Lu} &= 0.15 \frac{h}{\sqrt{\overline{(u'u')}_m}} \left(\frac{z}{h}\right)^{0.5} \\
T_{Lv} &= 0.07 \frac{h}{\sqrt{\overline{(v'v')}_m}} \left(\frac{z}{h}\right)^{0.5} \\
T_{Lw} &= 0.10 \frac{h}{\sqrt{\overline{(w'w')}_m}} \left(\frac{z}{h}\right)^{0.5}
\end{aligned}
\tag{8}
$$

where h is the height of the stable boundary layer.

In neutral conditions:

$$
\begin{aligned}
T_{Lu} &= \frac{0.5z}{1+15 \, {}^{fz}\!/_{u_*}} \frac{1}{\sqrt{\overline{(w'w')}_m}} \\
T_{Lv} &= T_{Lw} = T_{Lu}
\end{aligned}
\tag{9}
$$

where f is the Coriolis parameter and u_* is the friction velocity.

As early numerical simulations with the Langevin equation have shown, equation (1) is not suitable for inhomogeneous turbulent flows. In chapter 3 we will show that the ALPS model, when using only this basic Langevin equation theory, also gives incorrect results. In unstable conditions with vertical gradients of velocity variances, particles are trapped in areas of low variances. Those regions have small vertical dispersion, making it difficult for particles to move up/down and leave the area. This is why a number of scientists proposed the addition of a »drift correction« term to the Langevin equation (Rodean, 1996). Legg and Raupach (1982) introduced a vertical pressure gradient term, associated with the vertical gradient of vertical velocity variance. Thomson (1987) derived a more general criterion for stochastic Lagrangian models. The well-mixed criterion states that »if the particles of tracer are initially well-mixed they will remain that way«. Thomson also proposed a different scheme for the drift correction term. Rodean (1996) and Hsieh et al. (1997) cited that the model from Legg and Raupach (1982) does not satisfy the well-mixed criterion. Hsieh et al. (1997) have compared five different schemes for drift correction, including the ones from Legg and Raupach (1982) and Thomson (1987), in using a Lagrangian stochastic model for prediction of cumulative flux. They have found that all five models yielded very similar results. These results encouraged us to implement the

Legg and Raupach scheme for drift correction for now. The equation for subgrid-scale vertical velocity component is then:

$$w_r(t) = w_r(t - \Delta t)R_w(\Delta t) + w_s(t - \Delta t) + (1 - R_w(\Delta t))\, T_{Lw} \frac{\partial \sigma_{wr}^2}{\partial z} \tag{10}$$

where the third term on the right side represents the drift correction.

The drift correction is just one simple way of improving the treatment of convective conditions. More complex solutions consider the fact that the turbulence in unstable, convective conditions is non-Gaussian (Zannetti, 1990, Section 8.3.5; Rodean, 1996, Chapter 10). This is because vertical motion is organized into stronger and narrower updrafts and weaker but more widespread downdrafts. Some applications use two Langevin equations for updraft and downdraft, each with Gaussian forcing which results in an overall non-Gaussian turbulence (Baerentsen and Berkowicz, 1984 and Brusasca et al., 1987). De Baas et al. (1986) use non-Gaussian forcing for one Langevin equation. Luhar and Britter (1989) and Weil (1990) use a Langevin model with Gaussian forcing that is consistent with a known approximation of non-Gaussian inhomogeneous turbulence. We are aware that all these models give a better representation of turbulence in the convective PBL; however, because of the limitations of our project we choose to continue with only the drift correction term. We will show that it gives satisfactory results in unstable conditions for a simple application.

Trajectory integration algorithm needs the following fields imported from meteorological model: components of mean wind velocity u, v, w; turbulent fluxes $\overline{(u'u')}$,$\overline{(v'v')}$,$\overline{(w'w')}$, depth of mixing layer z_i, height of the stable layer h, and friction velocity u_*. It also needs decision algorithm for the planetary boundary layer (PBL) stability (stable/neutral/unstable) conditions. Three-dimensional fields of mean wind components over the whole domain are imported from meteorological model and then interpolated, using trilinear interpolation, to particle position. There are currently two options for determining the depth of mixing layer and stable layer: as the height at which turbulent kinetic energy (*TKE*) becomes smaller than some fraction of *TKE* maximum at the surface (currently 1/10 for unstable and 1/20 for stable conditions), or using vertical profiles of potential temperature θ (also imported from meteorological model) as the height of the first elevated stable layer. In simulations described in this paper the depth of PBL is determined using the potential temperature method. Turbulent fluxes are calculated from *TKE* interpolated from meteorological model. We emphasize that ALPS does not have its own turbulence parameterization and completely relies on the meteorological model regarding the structure of background turbulence. The friction velocity u_* is calculated from

$$u_* = \frac{k \cdot u(z)}{\ln(z/z_0)} \tag{10}$$

where k is *von Karman's constant* (k=0.4), $u(z)$ is wind speed at the height z, and z_0 is *roughness length*, set to 0.1 m due to the surface characteristics (Stull,1988). The stability is determined using vertical gradients of the potential temperature.

The model simulates the release of particles from multiple point sources. It can use complex topography, which is usually imported from meteorological model and interpolated to a particle position. Total reflection is applied at the surface. In order for ALPS to work in very complex topography, a specific algorithm for ground reflection was developed. When a particle is found to be below the interpolated ground elevation, it is reflected back along the path towards its previous position. The distance that it is reflected back equals two times the distance between the surface and the imaginary location of the particle below the surface. A coefficient which determines the probability of reflection at the top of the boundary layer is an input parameter. If the reflection at the PBL top occurs, the particle is vertically reflected downwards. Besides the change of the particle position, another important process occurs under reflection, both at the PBL top and at the ground. As stated in Zannetti (1990, Chapter 8), a change of sign of the »memory« of vertical subgrid-scale velocity component w_r is required. In the next chapter it will be shown that if the particle retains the same w_r towards the boundary, multiple reflections occur, resulting in unrealistically high particle concentration near the boundaries.

There is no deposition of particles and no chemical reactions in ALPS, as this project focuses on the basic numerical and dynamical properties of Lagrangian particle modelling.

The average concentration of the scalar represented by particles can be computed for arbitrary box area by keeping track of particles entering the area in the observed time and given the estimation of the emission rates.

3. Simulations

To show the behavior of the stochastic dispersion in different atmospheric stability regimes two simple idealized simulations were made. In both simulations the domain was flat with horizontal dimensions of 400 × 400 km^2, and the top of the domain was set to 4.3 km. Particles were emitted from a point source at the center of the domain with effective plume height set to 100 m above the ground. Mean wind velocity was constant and homogeneous, and set to u = 3 ms^{-1}, v = w = 0. Only between the first model level (at 10m above ground) and the ground velocity has logarithmic profile. Topography was removed from simulations to isolate the effects of turbulent diffusion in constant and simple wind field. At every timestep of 20 seconds, 20 particles were released and simulations were run for 5 hours.

3.1. Stable case

Vertical profiles of potential temperature θ and *TKE* representing statically stable stratification are shown in Figure 1a, where θ and *TKE* are horizontally homogeneous. While θ increases linearly with height, *TKE* has a maximum at the surface and decreases proportionally to z^{-1}.

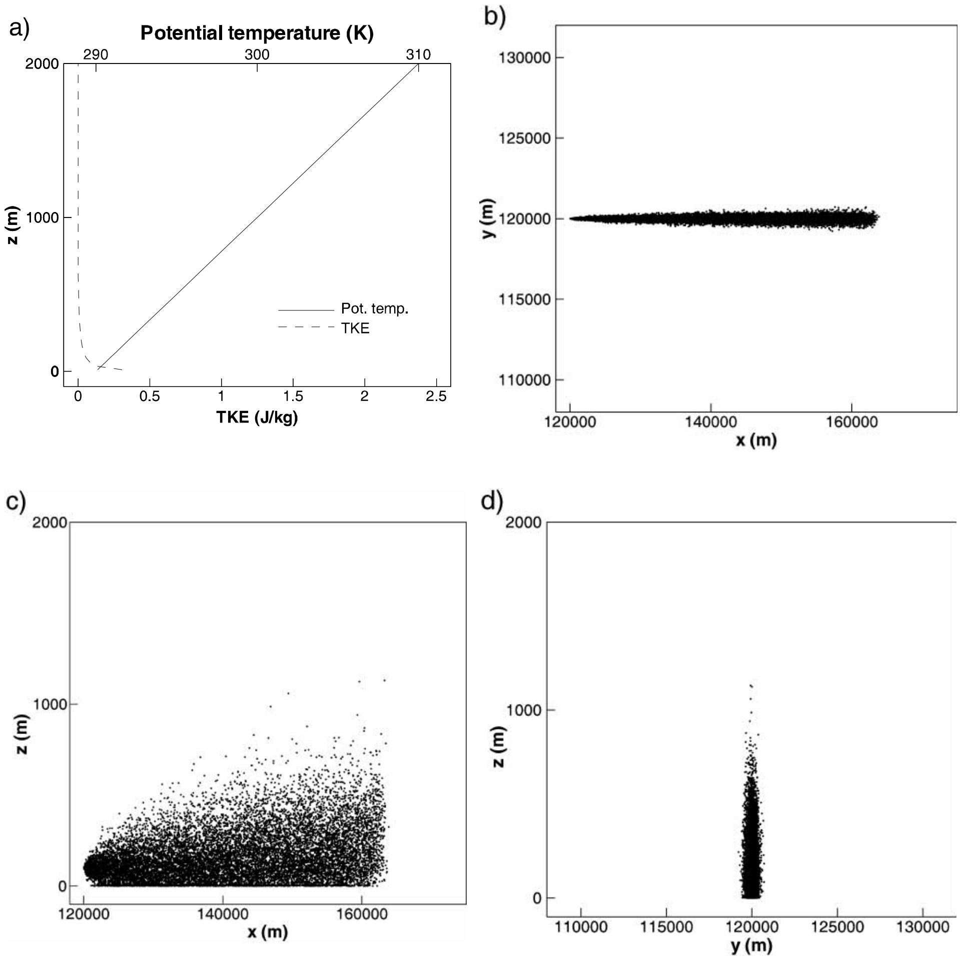

Figure 1. Vertical profiles of *TKE* and θ (a), X–Y (b), X–Z (c) and Y–Z (d) plane particle distribution for idealized test in stable conditions. The source is at x = 120000 m, y = 120000 m, z = 100 m; particle distribution is shown after 5 hours of integration.

Figure 1b shows the horizontal spread of the plume in X–Y plane. We can see that the particles are advected in *x* direction by the mean wind and not very dispersed due to weak turbulent fluxes. The spread of particles in horizontal is slightly stronger as the plume is advected farther from the source with concentration maximum always around the axis downwind from the source. Vertical distribution in X–Z plane is shown in Figure 1c. Again, the dispersion in the vertical is relatively weak (compared to unstable case) and gets stronger as particles travel away from the source. Maximum concentrations are between approximately 50 and 200 meters near the source, but the particles are more dispersed upwards as they move downwind because there is no reflection at the stable PBL top. The reflection was omitted deliberately, creating a situation where there is no exact boundary between stable PBL and free atmosphere, as can also be seen from θ profile. Figure 1d shows the form of the plume in Y–Z plane, perpendicular to the plume spread. It shows that the dispersion is quasi-symmetrical in horizontal, confirming normal distribution of stochastic subgrid-scale velocity components.

3.2. Unstable case

Figure 2a shows vertical profiles of θ and *TKE* near the surface in unstable atmospheric conditions. As in stable case, all meteorological conditions are horizontally homogeneous. The potential temperature decreases with height creating unstable conditions for the model up to 1250 m. Above that the atmosphere is stable. The *TKE* profile is typical for the unstable PBL, starting with ~0.5 m^2s^{-2} at the surface, increasing to maximum of 2.5 m^2s^{-2} at 300 m and then decreasing to zero at ~1500 m.

In Figure 2b horizontal distribution (X–Y plane) of the plume is shown. It can easily be seen that the horizontal dispersion is much stronger than in stable case (Figure 1b). Near the source concentration is greater around the center axis of the plume, but further downwind the dispersion distributes the particles more uniformly and the concentration decreases. Figure 2c shows the vertical distribution in X–Z plane downwind of the source. The particles are strongly dispersed in the vertical direction right after they are released from the source (bear in mind different scaling in *x* and in *z* direction). Total reflection is applied at the top of PBL. Very good uniform mixing is achieved away from the source. Figure 2d shows the plume in Y–Z plane. Cross-plume (Y direction) dispersion is uniform with height and concentration is highest on the central axis.

3.3. Conformity with the well-mixed criterion

As stated in the previous chapter, stochastic Lagrangian models must satisfy the well-mixed criterion. Figure 3 shows how ALPS was improved to achieve uniform concentrations through the whole depth of unstable PBL (unstable PBL has the most pronounced height variations in *TKE* and thus

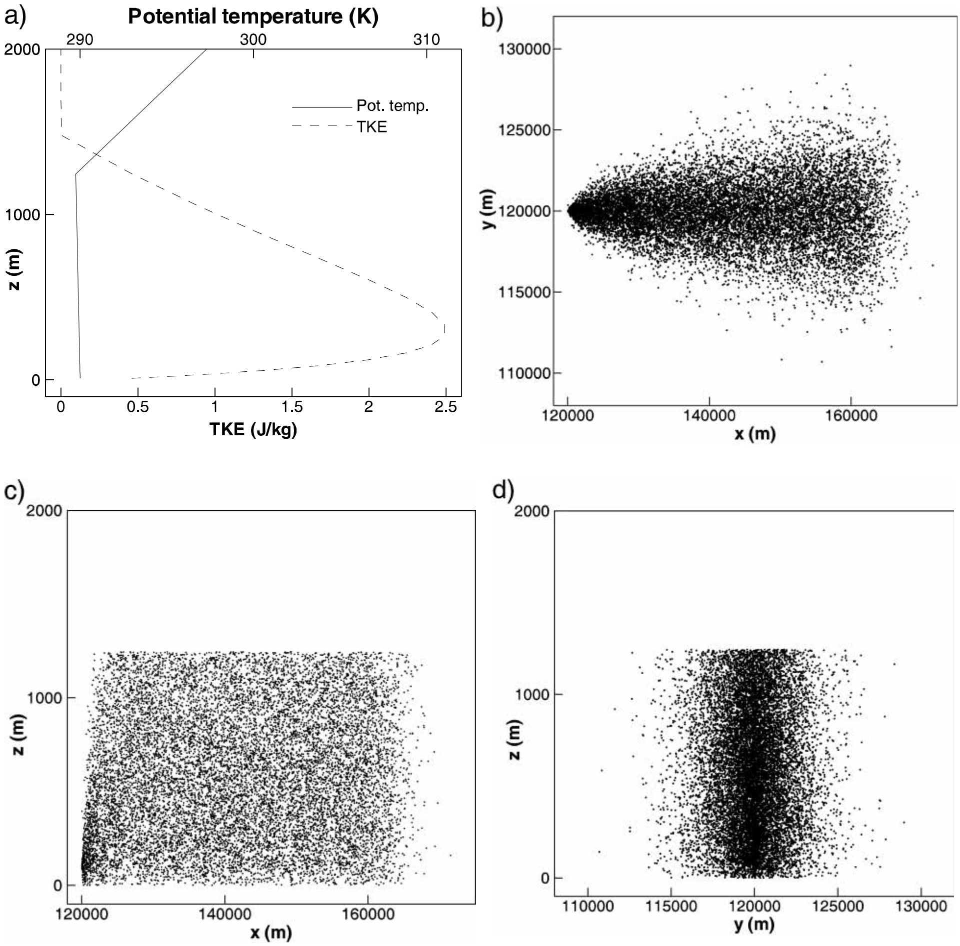

Figure 2. Same as Figure 1, except for unstable conditions.

in velocity variations). Simulation settings are the same as described for the unstable case. Figures show the particle distribution in the Y–Z plane, as in Figure 2d.

Two corrections are added to the model to obtain uniform mixing, as described in the previous chapter: a change of sign of w_r when reflection occurs (CS), and Legg and Raupach's drift correction term (LR). Figure 3a shows the case without both the CS and LR corrections. We can clearly see that the mixing is not uniform with height. Many particles are trapped in areas of low *TKE* (see Figure 2a). A small number of particles in the middle of the PBL results in small cross-plume dispersion. Mixing is improved when the CS correction is added (Figure 3b), although there are still increased concentrations

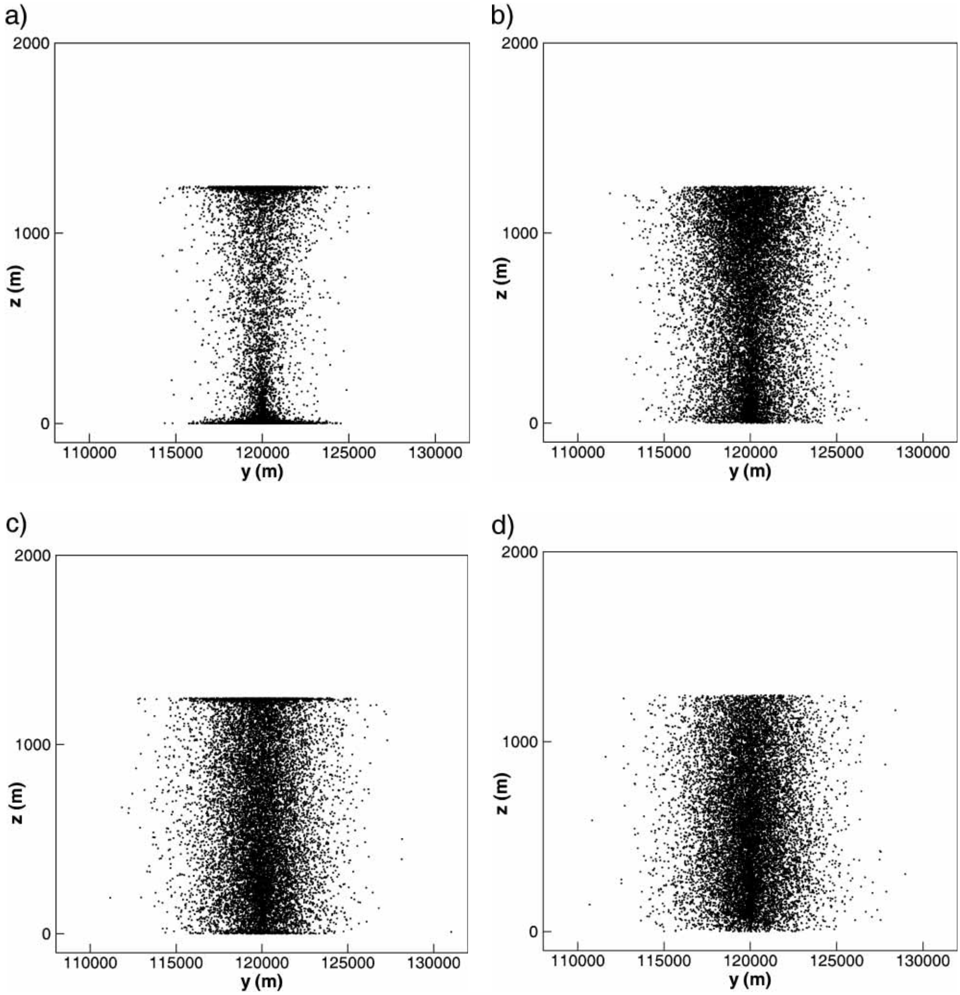

Figure 3. Y–Z plane particle distributions for idealized test in unstable conditions; without change of sign of w_r when reflection occurs (CS) and without Legg and Raupach's drift correction term (LR) (a); with CS and without LR (b); without CS and with LR (c); with both CS and LR (d).

near the ground and the PBL top. When we add the LR correction to simulation, but remove the CS correction (Figure 3c), there is better mixing in the middle areas of the PBL. But still, there are particles trapped in a narrow area close to the ground and the PBL top. Only when we add both the CS and the LR corrections to the model code (Figure 3d) are the particles well-mixed throughout the PBL (note: the slight increase in concentration in the lower half of PBL comes from the fact that this is not a Y–Z cross-section at some distance from the source but a particle distribution in Y–Z plane, showing also those particles that are very near the source; Figure 2d shows the same distribution in the X–Z plane, with completely uniform mixing at some distance from the source). Figure 4 shows the same simulations in the X–Y plane. Here we can see that adding the CS and LR corrections to the model also improves long-distance transport of particles and horizontal dispersion. In Figure 4a (without the CS and without the LR corrections) we see that the entrapment of particles also limits their horizontal movement. This happens because of multiple reflections at the ground which limit the particles' propagation and keeps them in the area of weaker mean-wind velocity (the logarithmic profile near the surface). Both the CS and the LR corrections individually (Figures 4b and 4c) contribute significantly to long range transport, and the combination of the two corrections (Figure 4d) produces slightly stronger dispersion.

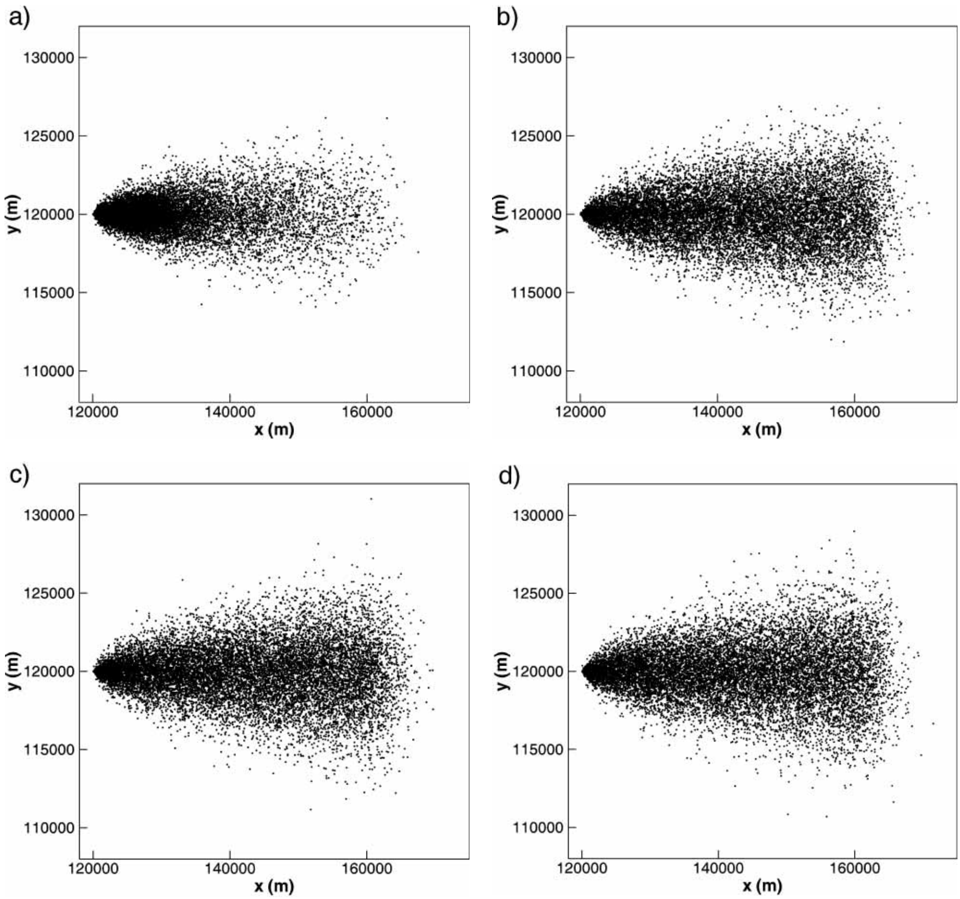

Figure 4. Same as Figure 3, except in the X–Y plane.

4. Conclusion

Initial development of the Atmospheric Lagrangian Particle Stochastic model ALPS was the subject of a graduate student project. Combining education and research, the project gave the students an insight to Lagrangian particle modelling and directions on how to apply obtained knowledge to practical purposes. The model is based on statistical approach and uses an Eulerian meteorological model output fields to estimate Lagrangian scales of turbulence. By calculating a large number (tens or hundreds of thousands) of particle trajectories it simulates the dispersion of a passive scalar in the atmosphere. The number of particles per unit volume is linearly proportional to scalar concentration at given time and position.

Some of its advantages over commonly used Gaussian models are: direct link of dispersion to the turbulence structure (no Gaussian assumption), the ability to work in extremely complex non-stationary, non-homogeneous and non-isotropic meteorological conditions and the ability to use very complex topography. The disadvantage might be its need for detailed meteorological information as well as the need to correctly link Eulerian and Lagrangian scales of turbulence. Also, Lagrangian particle models have greater computational cost compared to Gaussian models.

ALPS was built based on the same set of basic equations as in the LAP model from Koračin et al. (1998, 1999). However, all other issues in the model were left for the students to research and implement. ALPS depends on a meteorological model to provide the structure of turbulence. By conducting a series of idealized tests, it has been shown that ALPS correctly responds to different atmospheric stability conditions and their respective level of turbulence. The well-mixed criterion was met by adding a drift correction term to the vertical component of the subgrid-scale velocity. It is recognized that this is not a complete solution for all conditions in the convective PBL. The non-Gaussian nature of turbulence in convective conditions needs to be implemented in the model prior to any applications to experiments in such conditions.

The obvious next task is to compare ALPS against a proven Lagrangian stochastic model and validate it against tracer experiment data. With continuous improvements of model's trajectory dynamics, turbulence parameterizations, and concentration calculation, we believe that it will become a valuable contribution to air quality modelling studies.

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SAŽETAK

Edukacija i istraživanje: početni razvoj atmosferskog lagranžijanskog stohastičkog čestičnog modela ALPS

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Atmosferski lagranžijanski stohastički čestični model ALPS napravljen je kao eksperimentalni studentski projekt. Testiran je u idealiziranim i kompleksnim atmosferskim i orografskim uvjetima. Cilj projekta bio je studente direktno uključiti u najnovije znanstvene tehnologije. Model simulira disperziju pasivnog skalara u atmosferi tako da računa lagranžijanske trajektorije velikog broja čestica. Za srednje vrijednosti meteoroloških polja koristi rezultate meteorološkog modela. Za simulacije koristi prognostičku turbulentnu kinetičku energiju (TKE) iz nehidrostatskog meteorološkog modela višeg reda zatvaranja. Idealizirani testovi pokazali su da ALPS dobro reagira na različite uvjete statičke stabilnosti i povezuje disperziju čestica u zavisnosti o jakosti turbulencije, pri tome zadovoljavajući kriterij dobre izmiješanosti.

Ključne riječi: studentski projekt, modeliranje kvalitete zraka, idealizirane simulacije

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