Stochastic Lagrangian particle simulation of air pollution dynamic at mountain base and vicinity

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Abstract. In this work, we investigated the effect of horizontal turbulent diffusion coefficients on the pollution accumulation and distribution near the mountain. The diffusion coefficients, corresponding to variation of wind and particle flow, were considered in three different functions, which are constant, linear decay, and exponential decay function, in governing main simplified cases. In the calculation, the transport of pollution was performed using Lagrangian particle models. The results show that the characteristics of pollution distribution were given by how diffusion coefficients are functioned. Specifically, the non-variant of turbulent diffusion coefficient causes the pollution concentration to get highly accumulated close to the mountain boundary. However, the higher magnitude in non-variant diffusion coefficients allows more turbulences and reflect the highest pollution concentration to step away from the mountain base. Nevertheless, for diffusion coefficient in variant version, the pollution distribution characteristic lies between the low and high non-variant limits, caused by the decay of the diffusion coefficients away from the mountain. However, the exponential decay tends to spread the pollution further out than that of the linear decay due to the abrupt drop of the diffusion coefficients.

1. Introduction

The enhance of economic growth via industrial development usually delivers pollution in the areas as its by product. If the management to eliminate this pollution does not function properly, the leak of pollution may propose some risks on people health living in that area. However, due to specific characteristic of the geographic regions and the dynamic change of construction making by human, how to plan for pollution confinement for later elimination is somewhat difficult to handle. Therefore, it is of great interest to develop models that can not only adapt to the considered geographic geometries but also handle the dynamic changing of the air flowing above the regions. From literatures, there were the numerical models proposed to predict dispersion of pollution in atmosphere, which are useful for the planning of countermeasures [1]. However, previous models usually scoped on the pollution convection and diffusion from the emission sources, with an emphasis on horizontal directions of pollution spreading out [2]. The Lagrangian particle model has been usually used to compute the trajectories of substantial number of atmospheric particles. One advantage of using Lagrangian model is that it is independent from the computational grid and does not need to solve differential equation as in the Eulerian model [3]. In a recent work, the stochastic Lagrangian particle model considered turbulent diffusion coefficients being constants in the horizontal directions because the studied region was set in urban [4]. However, for the region closed to the obstacle, such as being situated near a mountain, the coefficients should be spatially dependent and more complex turbulent diffusion parameters should be taken into account around the foothill [5, 6]. Then, the turbulent diffusion coefficients in horizontal direction near the mountain base should not be constant as in the previous urban area studies. Therefore, in this study, the turbulent diffusion coefficients in horizontal directions (K_x and K_y) have been varied in the area close to the mountain-like obstacle, as the 'mountain' does obstruct and distorts the pollution transportation path from its ideal flow. There distinct functions were considered for the variation of the K_x and K_y near the foot hill.

2. Materials and methods

In this work, stochastic Lagrangian particle model was used for simulating the pollution distribution on local scale because this model can handle high gradient of pollution near the point source. The particle density represents a given concentration and can be moved in 3D space by advection and turbulent diffusion. As advection field is deterministic, but the effect of the turbulent diffusion is stochastic, the particles flow to new positions which can be calculated from [1]

$$X_{new,i} = X_{old,i} + v_{adv,i}dt + \bar{x}_i \, , \tag{1}$$

where $X_{new,i}$ and $X_{old,i}$ are the spatial coordinates of particles after and before the flow, respectively. $v_{adv,i}$ is the i^{th} coordinate of the wind velocity vector, and dt is the time step. The last term in equation (1), i.e. $\bar{x}_i$, describes the effect of stochastic turbulent processes, and i denotes the index of spatial Cartesian dimension (i = 1, 2, 3). This stochastic term can be calculated from $\bar{x}_i = r\sqrt{2K_i dt}$, where random numbers r take on normal distribution with zero mean and a unit variance, which were generated using Mersenne Twister random number generator [7] and a Cartesian Box–Müller transformation [8]. $K_{x(y)}$ are horizontal turbulent diffusion coefficients, and vertical diffusion coefficient K_z is

$$K_z(z) = \frac{ku^* z}{\Phi(z/L)}\left(1 - \frac{z}{H_z}\right)^2 . \tag{2}$$

In equation (2), k, u^*, H_z, $\Phi(z/L)$ and L are von Kármán's constant, friction velocity, mixing layer height, similarity function for heat and Monin–Obukhov length, where z is the height of interest. Friction velocity and Monin–Obukhov length were calculated iteratively as a function of the actual vertical stratification of the atmosphere [9]. The studied domain took a size of 40 km × 40 km × 300 m with the mountain situating at the top-left of the domain as shown in figure 1(a). The pollution emission source was located near the left bottom and the average wind direction was set from south to north with wind speed of 1 m/s. The turbulent diffusion coefficients K_x and K_y were varied from 1000 m^2/s to 10000 m^2/s (in magnitude) within the range 5 km away from the mountain boundary. Constant, linear decay and exponential decaying functions were used for K_x and K_y variation near the mountain as shown in figure 1 (b). The non-variation version (constant version) of K_x and K_y was included in the simulation to compare with the variational ones. The particles that fly across the domain boundaries are no longer included in the calculation as they are now lying outside the considered regions.

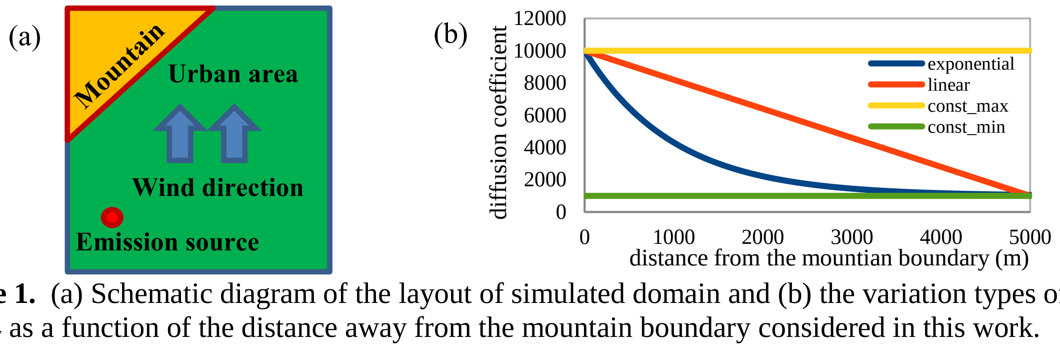

Figure 1. (a) Schematic diagram of the layout of simulated domain and (b) the variation types of K_x and K_y as a function of the distance away from the mountain boundary considered in this work.

3. Results and discussion

In this study of pollution transport simulation, the pollution was emitted from a point source for duration of 24 hours. The wind field direction was directed towards the mountain from south to north during the simulation. At first, the distribution of particle was studied when the turbulent diffusion coefficients K_x and K_y were set constant at 1000 m^2/s for the whole entire simulated domain. The pollution particles were found to highly concentrate at the mountain base as shown in figure 2(a), as the particles hardly change their motion direction away from the wind direction and get accumulated at the mountain boundary. However, when K_x and K_y were changed to 10000 m^2/s, particle distributes differently from the previous low K_x and K_y case as shown figure 2 (b). The highly concentrated region was found further away from the mountain base, where close to the mountain base, there is very low particle concentration. This low concentration near the mountain base may be due to the wind advection, normally blowing towards and reflecting off the mountain, is subjected to heavily turbulent effect which changes the ordinary wind field directions to random ones in this region. Therefore, the accumulation of particles flowing into the region tends to step away from mountain base with some distances. For K_x and K_y decaying as a linear function away from the mountain base, the particle distribution is qualitatively similar to high constants K_x and K_y case, but the highly concentrated line is broader and position further away from the mountain base. To explain, the linear decreasing of K_x and K_y lessens the turbulent effect on the wind field direction, which may somewhat allow the wind to keep its direction towards the mountain base. However, when the particle is flowing near the mountain base, the wind advection still experiences some strong turbulent influences and wind direction may amend randomly. Therefore, the particle accumulation in this linear case shows mixing characteristics between low and high constants K_x and K_y cases. Finally, for the K_x and K_y in the form of exponential decay function, it shows even broader of highly concentrated region near the mountain base. In this case, the K_x and K_y slowly change at distances far away and abruptly increase near the mountain base, which cause the wind field direction in this region gradually but randomly change from the ordinary direction. This is partly like the linear case, but particles get accumulated nearer to the mountain base, giving more dispersive pattern.

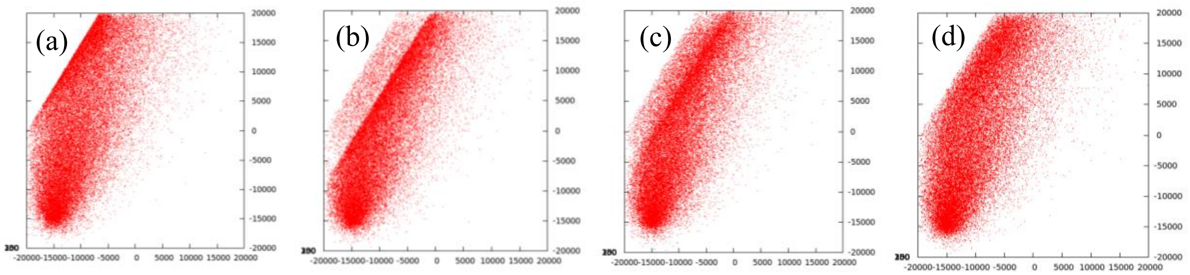

Figure 2. Particles distributions when K_x and K_y are (a) 1000 m^2/s, (b) 10000 m^2/s (c) linear decay function, and (d) exponential decay function.

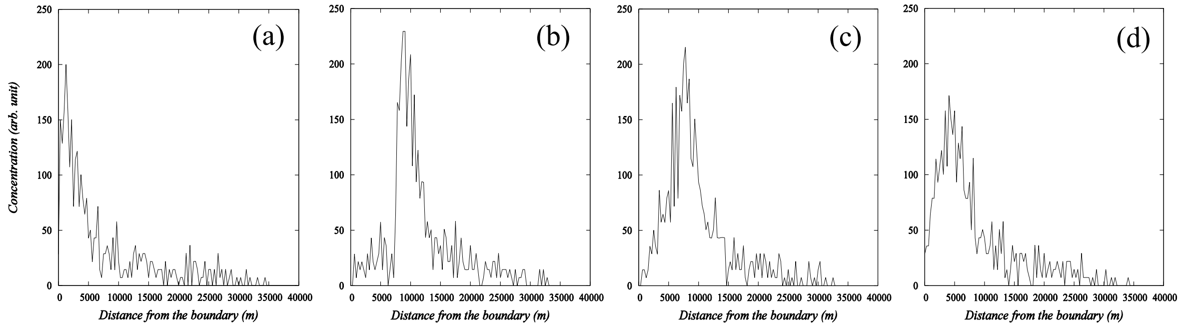

Figure 3. Pollution concentration as a function of distance when K_x and K_y are (a) 1000 m^2/s, (b) 10000 m^2/s (c) linear decay function, and (d) exponential decay function.

Next, when plotting the concentration as a function of distance away from the mountain base, for $K_x = K_y = 1000\ m^2/s$, we could see that the concentration is highest at the distance of 2 km away from the base as shown in figure 3(a). Away from the mountain, the concentration increases along the way towards the boundary but sharply drop at a distance very close to the base due to particle being bounced back from the mountain. Then, when considering the case of $K_x = K_y = 10000\ m^2/s$, as shown in figure 3(b), the highest concentration peak exists at about 10 km away from the base. Specifically, the concentration rapidly increases on moving towards mountain base and then abruptly drops, which are due to that the high turbulence causes the particle to spread out of the region near the mountain. The low concentration within the region near the mountain suggests that the particles can either flow out of region or get deposited at the boundary which yields the high concentration at or close to the mountain base. For K_x and K_y varying as a linear and exponential decay function, the exponential K_x and K_y yields broader region of high concentration area than that of the linear K_x and K_y as shown in figure 3(c,d). The highest concentration peak of linear K_x and K_y exists at about 8 km away from the mountain base, whereas the exponential K_x and K_y results the peak closer to the mountain at the distance about 5 km. In addition, the distribution peak of the exponential is less in magnitude compared with the linear one due to the greater level of dispersiveness in pollution distribution. In summary, when considering all considered K_x and K_y cases, in term of pollution concentration peak as a function of distance away from the mountain, the linear K_x and K_y case yields the farthest distance where the constant $K_x = K_y = 1000\ m^2/s$ yields the nearest distance, which are somewhat extreme circumstances. Including with the irregular accumulation of the pollution (see figure 3), the exponential decay in K_x and K_y seem to be the most natural dispersion of the pollution near the mountain boundary than the other kinds considered in this work.

4. Conclusion

This work used stochastic Lagrangian particle model to simulate the pollution transport in the vicinity of mountain base, where the turbulent is more complex compared to the plain geography in urban region. The three kinds of functions, which are constant function, linear decay function, and exponential decay function were used as the variation model of horizontal turbulent diffusion coefficients along the *xy* directions, i.e. K_x and K_y. The results show that the variations of the horizontal diffusion coefficients yield the different characteristic of the air pollution distribution near the mountain. Their pollution concentration distribution occurs differently in each function type. In the constant function, the high constant case yields the highest pollution concentration to position furthest away from the mountain, whereas the highest concentration of the exponential function exists nearest to the mountain base. Moreover, the broadness of high concentration peak is greatest in the exponential function but narrowest in the high constant case. Therefore, which these concentration distribution characteristics associated to variation of K_x and K_y near and at the mountain base, we could simply implement one of them that is most appropriate to the terrain of interest to predict the pollution distribution in the areas.

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