Diffusion Process of Aerosol Particles with Different Diameter over Complex Terrain

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ABSTRACT

Properties of the aerosol particle (AP) is important to understanding the formation of fog-haze, and even for the evolution of climate. Based on the mesoscale large-eddy simulation model of ARPS and with the consideration of gravitation deposition (GD), the diffusion process of AP with three diameters of $10\,\mu m$, $50\,\mu m$ and $100\,\mu m$ over complex terrain are investigated. Simulation results show that the diffusion of AP with different diameter exist differences and universality. For the AP with smaller diameter of $10\,\mu m$, the diffusion range along stream direction and height is very large due to the stronger fluid following and the slight GD properties. While for the AP medium diameter of $50\,\mu m$, the diffusion range along stream direction decreases rapidly but less changed along height. Under the strongly GD effect, the diffusion range of AP with diameter of $100\,\mu m$ along two direction is very small. For all AP with different diameter, the diffusion height trends to a steady state and exist a “overshoot” phenomenon obviously.

Key words: Aerosol particles (AP) diffusion, large eddy simulation (LES), complex terrain, gravitation deposition (GD).
1. INTRODUCTION

The artificially and naturally emissions of aerosol particles (AP) increase with increasing the nature developed by human. The evolutions of AP have significant influence on the global climate changed and the natural disasters such as sandstorms’ happened [1, 2].

The high concentration of AP not only affects the natural environment, but also endangers human’s health [3]. The diffusion and emission of AP in global and region were studied by large plenty of researchers [4-6], and many prediction systems such as Weather Research and Forecasting (WRF) [7] and Advanced Regional Prediction System (ARPS) [8] were established. However, the weather data such as wind field were needed to support these existing patterns. Therefore, the precision of prediction patterns was determined by the time-space resolution and ground characteristic. While the prediction precision of AP diffusion for the complex terrain, is relative poor due to the lack of real-time meteorological data. So it is vital to investigating the diffusion mechanisms of AP with different diameter under the complex terrain. The diffusion process of AP is closely dependent on the wind field. So the precision simulation of wind field is the key. At present, three methods of direct numerical simulation (DNS), large eddy simulation (LES) and Reynolds Averaged Navier-Stokes (RANS) are mainly included. DNS is used to study the microscopic mechanism of turbulence flow due to its huge calculation. And the momentary flow can’t be obtained by RANS [9, 10].

In this study, wind field is simulated based on LES. Firstly, simulation model of complex terrain with the gravitation deposition taken into account is established. And then the diffusion distance of AP along stream and height with different mass concentration is analyzed. Finally, comparison the diffusion evolution of AP with different diameters and discussion their difference and similarity are given.

2. MODEL AND METHOD

2.1 Wind field

In this study, the mesoscale large-eddy simulation (LES) model of ARPS is used, and then the internal diffusion functions of AP in the model are modified. The solution of wind field can be obtained based on the three-dimensional and fully compressible Navier-Stokes equations. The continuity and momentum conservation government equations can be written as [11]

\[
\frac{\partial \rho \bar{u}_j}{\partial t} + \sum_{i=1}^{3} \frac{\partial \rho \bar{u}_i \bar{u}_j}{\partial x_i} = - \frac{\partial \tau_{ij}}{\partial x_j} - \frac{\tau_{ij}}{\partial x_j} + \frac{\partial S_i}{\partial x_j}
\]

where \(\bar{ }\) means the filtered variables, \(i = 1, 2, 3\) indicate coordinates of the
streamwise, spanwise and vertical directions, respectively, $u_i$ is instantaneous velocity component, $\overline{\rho}$ stand for the volume mean air density, $t$ means time, $\tau_{ij}$ is the air viscous stress, $\delta_{ij}$ means the Kronecker delta, $\rho' = \rho - \rho \overline{\rho}$ is the disturbance pressure, $\alpha$ means the damping coefficient, $B = -g \rho'/\overline{\rho}$ is the buoyant caused by the density $\rho'$ changes, $g$ is the gravitational acceleration.

The subgrid stress tensor caused by the filter operation is $\tau_{ij} = \rho \mu' u_i u_j - \rho u_i u_j$, which character the influence of vortex less than the grid scale on the flow, and can be determined by the formula according to Smagorinsky (1961):

$$\tau_{ij} = -2(C_s \Delta)^2 \left[ \overline{S} \right] \overline{S}_{ij}$$

where $C_s$ is the Smagorinsky coefficient, $\overline{S}_i = (\partial \overline{\rho} / \partial x_i + \partial \overline{\rho} / \partial x_i) / 2$ stand for the strain rate tensor, $\Delta$ is the filter scale, $\left[ \overline{S} \right] = \sqrt{2 \overline{S}_i \overline{S}_{ij}}$ is the strain rate. Here, the dynamic Lagrangian subgrid model for the complex terrain is adopted (Meneveau et al., 1996).

### 2.2 Diffusion and deposition equation of aerosol particles

Variations of AP concentration obey the components mass conservation and can be formulated as $^{[12]}$

$$\frac{\partial \rho c}{\partial t} + \frac{\partial}{\partial x_i} (\rho u_i c) = \frac{\partial}{\partial x_i} (K_i \frac{\partial c}{\partial x_i}) - S_c$$

where $c$ means the volume concentration of AP, $K_i$ ($i = 1, 2, 3$) are respectively the diffusion coefficients along three direction and can be expressed by the form $^{[13]}$:

$$K_i = K_{i0} \sqrt{1 + \left( \frac{\beta w_i(d)}{\sigma} \right)^2 - \frac{1}{2} \left( \frac{\beta w_i(d)}{\sigma} \right)^2}$$

$$K_s = K_{s0} \frac{1}{1 + \left( \frac{\beta w_i(d)}{\sigma} \right)^2}$$

In which, $K_{i0}$ and $K_{s0}$ are respectively the diffusion coefficients along horizontal and perpendicular direction, $w_i(d)$ means the terminal deposition velocity of AP with diameter $d$, $\sigma$ and $\beta$ stand for the parameters dependent on wind field, respectively.
2.3 Computational settings and boundary conditions

One mountain in northwestern China was selected in this study, where the latitude and altitude are $E86^\circ 49'$ and $N43^\circ 06'$, respectively. The terrain data is taken from a DEM database with a resolution of 30m. The average altitude is about 4000 meters, and there exist 800 m distance between the highest and the lowest land, as shown in Fig. 1(a).

Here, the computational domain is set to be $5km \times 3km \times 3km$, and the horizontal grid numbers are $n_x = 50m$. The grids along perpendicular are stretched and the minimum values are $n_{z_{\text{min}}} = 5m$. Simulation model is presented in Fig. 1(b).

To investigate the influence of AP diameters on their diffusion evolution, three diameters of $10\,\mu m$, $50\,\mu m$, and $100\,\mu m$ are selected. The initial wind field is set as homogeneous profile and the boundary layer depth is 500 m. The neutral atmosphere is modeled. Here, the rigid boundary condition is set at the ground, and the open radiation boundary conditions are selected along the lateral and the top boundaries. Simulation process is divided into two stages. The first stage is the development of flow field and the second stage is the investigation of diffusion evolution after the emission of AP.

![Figure 1. (a) Contours map of computational terrain and (b) schematic of the grid.](image)

3. RESULTS AND DISCUSSIONS

3.1 Wind field analyses

Wind compression simulation is the foundation of the prediction of AP diffusion process accurately. Based on the LES and with the high accuracy grids included, the wind field and flow structure with small scale over complex terrain can be simulated precisely. Fig. 2(a) present the wind vector at the ground of 5m after 10 hours. Where the wind direction is southeast and the initial wind speed is 2m/s.
Figure 2. (a) Vector map of wind field at the ground of 5m and (b) comparison of the simulation results with the experimental data for the wind acceleration ratio.

Seen from Fig. 2(a), it can be found that amount of turbulent vortexes that flow around the terrain will be occurred, especially for the wind magnitude and direction near ground. Meanwhile, there appears a lot of accelerate effect of windward and circulation of terrain. To verify the simulation wind field, the wind distribution along the windward (seen the red triangle in Fig. 2(a)) is obtained. Here, the measurement distance is set as 100m. Comparison of the simulation results with the experimental data for the wind field presented in Fig. 2(b) is consistent with each other. In addition, a fluctuating phenomenon, which may stem from the local micro terrain, is observed in the simulation.

3.2 Diffusion process of aerosol particles

In this section, continuous emission of AP are set at the media point of the windward slope in the southeast region firstly, where the distance from east and south are respectively 500m and 1000m, as shown in Fig. 1. Here, the flow direction is set as southeast, the computation domain is initialized with the uniform velocity of $6 m/s$ and the emission rate is $50 \text{ mg/s}$. The flow development time is two hours and then AP is released.
Fig. 3 shows the mass concentration cloud map of AP with the diameter of $10\mu m$, where (a), (b) and (c) are the emission after half, second, and eighth hour, respectively. It is found that AP spread rapidly along stream with emission, and AP exhibits a better following feature due to their small diameter. After two hours emission, AP has flied off from the computation region. It can also be found that the development of AP in high concentration is so slowly, and even tend to be stable during a period of emission. To better understand the diffusion feature of AP with diameter of $10\mu m$, Fig. 4 present its statistical results at different concentration region.

Seen from Fig. 4, it can be found that the diffusion distance decreases with increasing the mass concentration, and then tend to stability for the high concentration. And for the largest diffusion distance of AP with the mass concentration of $5.0 \text{ mg/m}^3$ and $10.0 \text{ mg/m}^3$ are respectively $1200m$ and $650m$ along stream, $250m$ and $200m$ along height. Therefore, the diffusion distance for small AP such as the diameter of $10\mu m$ and below it always keeps a stable level under the continuous emission. The main reason for that is the mass concentration of AP decreases with increasing the diffusion distance due to their deposition, and then comes to dynamic balance due to the continuous emission and deposition. Meanwhile, the diffusion distance of the low mass concentration is so larger.
Figure 4. Variation of the largest diffusion distances of AP with diameter of 10 \( \mu \text{m} \) versus time along the (a) stream and (b) height under three mass concentrations (0.1, 5.0, and 10.0 mg/m\(^3\)).

The mass concentration cloud maps of AP with the diameter of 50 \( \mu \text{m} \) under east wind after emission of the first, second, and fifth hour are presented in Fig. 5(a), (b) and (c), respectively. Where the cloud map at upper row is the top view and height color map at bottom row is the corresponding mass concentration. It is found that the diffusion distance of AP with diameter of 50 \( \mu \text{m} \) is smaller than that of small particle with diameter of 10 \( \mu \text{m} \), especially along stream direction. However, seen from the height cloud map, the achieved height of AP with diameter of 50 \( \mu \text{m} \) is far greater than that along stream. The reason for that is the stronger rising airflow. After about five hours, AP is perforated from the top boundary along height. It can also be found that the diffusion velocity is still so slow for the high concentration region.

The variation of diffusion distance of AP with diameter of 50 \( \mu \text{m} \) versus time is presented in Fig. 6. It can be found that the largest diffusion distance of AP with diameter of 50 \( \mu \text{m} \) along stream is limited, they all deposition when the distance comes to 2000m. Therefore, the stream diffusion distance will keep a constant state under the effect of deposition for the AP diameter comes to 50 \( \mu \text{m} \), while fast spread along height and pass through the computation area after 4 hours emission. Comparison the diffusion process of AP with diameter of 10 \( \mu \text{m} \), the diffusion rate along height is close to AP with diameter of 50 \( \mu \text{m} \). The main reason for that is the stronger turbulence diffusion at the height. Where the largest diffusion distance of AP with mass concentrations of 0.5 mg/m\(^3\), 5.0 mg/m\(^3\), 10.0 mg/m\(^3\) are about 2000m, 500m and 250m along stream, respectively. And are 3000m, 250m and 200m along height. One interested phenomenon that the variation of diffusion distance of AP with different mass concentration appear a “overshot”, which reaches a larger value first and then tend to be stable.
Figure 5. Mass concentration cloud map of AP with the diameter of $50 \mu m$ under east wind after emission of the (a) first, (b) second, and (c) fifth hour.

Figure 6. Variation of the largest diffusion distances of AP with diameter of $50 \mu m$ versus time along the (a) stream and (b) height under three mass concentrations (0.1, 5.0, and 10.0 mg/m$^3$).

Fig. 7 presents the concentration contour of AP with the diameter of $100 \mu m$ under east wind after emission of the first, third, and fifth hours, respectively. It can be found that the diffusion distance of AP reduces significantly due to the obvious deposition effect for the large AP. In fact, the particle with the diameter of $100 \mu m$ is not belong to AP. Here, the largest diffusion distances of AP with $100 \mu m$ diameters along the stream and height for three diameters are still analyzed. Meanwhile, to see the comparisons more clearly, the results of AP with diameters of $10 \mu m$ and $50 \mu m$ are shown in the same Fig. 8.
Figure 7. Mass concentration cloud map of AP with the diameter of 100 $\mu$m under east wind after emission of the (a) first, (b) third, and (c) fifth hour.

Figure 8. Variation of the largest diffusion distances of aerosol particles versus time along the (a) stream and (b) height for three diameters (10, 50, and 100 $\mu$m) and three mass concentrations (0.5, 5.0, and 10.0 mg/m$^3$).

It is found that the diffusion distance for the small AP is larger than the large under constant emission of AP, while didn’t dependent on the AP diameters for the high concentration area. And the influence range such as the concentration is larger than 5.0 mg/m$^3$ tend to stability. The concentration decreases with increasing of AP for the same diameter.

4. CONCLUSION

Based on the compressible fluid large eddy simulation (LES), the evolution of aerosol particles (AP) diffusion with three diameters of 10 $\mu$m, 50 $\mu$m and 100 $\mu$m are investigated in this paper. The main conclusions are as follows:

(1) Under the steady emission of AP, the high ranges of AP with different diameters tend to be stable and they all exist obviously “overshot” phenomena.
The diffusion range of AP is inversely proportional to the AP diameter. That is, the smaller diameter of AP, the smaller its range of AP.

For the small AP, the diffusion along the high is affected by the turbulence greatly.

There still need some improvement. For example, the small computation domain is selected for the precision of the wind field, which leading to the overall diffusion process of the smaller AP can’t be studied. Meanwhile, the comprehensive investigation on the diffusion of AP is not discussed due to smaller kinds of AP diameters.

REFERENCES