Numerical Investigation of the Diffusion Feature of Aerosol

Zhengshi Wang, Shuming Jia and Shumin Li*

ABSTRACT

High concentration aerosol solid particle affect human health seriously. The transportation and diffusion processes of mid-air aerosol are vital to the understanding of the formation and evolution of fog-haze. Based on the mesoscale large-eddy simulation model ARPS and introducing atmosphere turbulence, the diffusion process of aerosol under different conditions is investigated. The results indicate that pollution diffusion in calm atmosphere is a rather slow process, while convection can push the pollution towards downwind effectively. Turbulence can affect the diffusion process profoundly and enhance the diffusion velocity largely. In the process of wet scavenging of aerosol particles, atmosphere turbulence increases the treating limits effectively but decreases the local efficiency to a certain extent.

Key words: Aerosol, diffusion process, atmosphere turbulence, wet scavenging.

1. INTRODUCTION

With the rapid development of global industrialization and economy, the growing air pollution problems (e.g. haze-fog) have drawn more and more attention [1, 2]. Aerosol is a suspension system that composed of small solid

State Key Laboratory of Aerodynamics, China Aerodynamics Research and Development Center, Mianyang, Sichuan 621000, China
Computational Aerodynamics Institute, China Aerodynamics Research and Development Center, Mianyang, Sichuan 621000, China
*Corresponding author Email address: lishmin17@cardc.cn
particles in the air, which is an important source of material to form fog-haze days \cite{3, 4}. Fog and haze not only affect the visibility and human health, but also influence the climate profoundly through absorbing and reflecting solar radiations \cite{5, 6}.

Large plenty of researches have been conducted for the purpose of understanding the size distribution and components \cite{7, 8}, optical characteristics \cite{9, 10}, and physicochemical properties of aerosol particles \cite{2, 11}. The transportation and diffusion of aerosol is vital for the prediction of affected area and the exploration of the emission source. Although several researchers have investigated the transport of aerosol through the gas tracking method, there is still lack of the comprehensive study of the diffusion pattern of aerosol, especially under the condition of atmospheric turbulence.

Based on the mesoscale atmosphere prediction pattern of ARPS (Advanced Regional Prediction System), the diffusion process of pollution under calm and turbulent air is respectively investigated. The diffusion velocity and the influence of atmospheric turbulence on the diffusion process are mainly discussed. At the same time, as one of the most common method that can eliminate aerosol particles, the efficiency of wet scavenging under diffusion and convection are also explored.

2. MODEL AND METHOD

2.1 Governing equations

The three dimension non-hydrostatic compressible LES model of ARPS is used to predict the atmospheric flow \cite{12, 13}. The density of moist air can be written as:

\[ \rho = p(1 - q / (\varepsilon + q)(1 + q)) / (R_d T) \]  \hspace{1cm} (1)

in which \( p \) is the air pressure, \( q \) is the water vapor mixing ratio of air, \( T \) is the air temperature, \( R_d \) is the gas constant of dry air, \( \varepsilon = R_d / R_v \) and \( R_v \) is the gas constant of vapor.

The filtered continuity equation, momentum conservation equation and scalar diffusion equation can be expressed as:

\[ \frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i} (\rho u_i) = 0 \]  \hspace{1cm} (2)
\[
\frac{\partial}{\partial t}(\rho \tilde{u}_i) + \frac{\partial}{\partial x_j}(\rho \tilde{u}_i \tilde{u}_j) = -\left(\frac{\partial p^*}{\partial x_i} + g \rho' \right) - \frac{\partial}{\partial x_j} \left( \mu \frac{\partial \tilde{u}_i}{\partial x_j} \right)
\]

in which the tilde and apostrophe represent filtered and perturbation variables, respectively. \(x_i\) and \(u_i\) are the position coordinates and instantaneous wind speed components along streamwise \((i = 1)\), spanwise \((i = 2)\) and vertical directions \((i = 3)\), respectively; \(t\) is time and \(p' = p - \alpha V(\rho u)\) include the pressure perturbation and damping item, and \(g\) is the gravitational acceleration.

In equation (4), \(\phi\) represents scalar variables and can be temperature, water substances (vapor, cloud water, rain water, etc.) or pollution concentration. And \(S_{\phi}\) is the corresponding source item.

2.2 Model settings

The computational domain is \(100 \times 100 \times 100\) m in this study. The horizontal grid size is uniform and equals to 1.0 m. While the vertical grid is stretched with an even grid scale of 0.5 m in the range of 0–20 m, the grid ranges from 20 m to 50 m is stretched and above it is unified grid size. The mean grid size is also 1.0 m along vertical direction.

Open radiation boundaries is used for the around boundaries. The bottom is rigid wall and the top uses the free slip boundary combined a Rayleigh damping layer of 20 m. The large and small time step are 0.05 s and 0.001 s, respectively, and the total simulation time is 30 minutes. The initial potential temperature and relative humidity of the air is 300 K and 60\%, respectively.

3. RESULTS AND DISCUSSION

3.1 Diffusion features of aerosol

Convection and diffusion is the two major form of aerosol transport, in which convection refers to the aerosol travelling along downwind, and diffusion means pollution transfers form high concentration zone to low
concentration zone spontaneously.

In order to observe the diffusion and convection of aerosol in the air directly, the evolution of an ellipsoidal concentration bubble is firstly performed. As shown in Fig. 2, the first row shows the diffusion process concentration bubble under calm atmosphere, and the second row gives the concentration evolution process under a wind speed of 1m/s. Seen from the figure, the diffusion of aerosol particle under (quasi) calm atmosphere is a rather slowly process, and its diffusion velocity decreases with time due to the smaller concentration gradient.

![Figure 1. Evolution of the concentration bubble under calm air and breeze (U=1m/s).](image)

(Initial condition: the ellipsoidal concentration bubble is located at $x = 50m$, $y = 50m$ and $z = 5m$, the half axis are respectively $a = 10m$, $b = 10m$ and $c = 5m$, the initial mass concentration is $500 \mu g/m^3$. The wind direction is form left to right under breeze, the free stream velocity is 1.0m/s and obeys the logarithmic profile, and the boundary layer depth and roughness height are respectively 50m and 0.01m.)

However, under the actions of wind, the efficiency of convection is more remarkable than that of the diffusion effect. From the figure, high concentration bubble shifts towards downward, and diffuses slightly during this process, the move velocity of the bubble is consistent with the wind speed.

Fig. 3 shows the diffusion velocity of concentration versus time, in which the black and green lines represent the domain with mass concentration larger than $1 \mu g/m^3$ and $50 \mu g/m^3$, respectively. It can be found that the diffusion velocity of low concentration domain is larger than that of high concentration domain. After half an hour, the high concentration domain ($50 \mu g/m^3$) expends
about 3m and its diffusion velocity decreases from approximately 10cm/min to 0.2cm/min.

![Graph showing diffusion velocity vs. time](image)

Figure 2. Evolution of the diffusion velocity of concentration bubble versus time under calm air (the diffusion velocity is the mean value of the diffusion velocities along four horizontal direction).

Since atmospheric turbulence directly influences the diffusion velocity of aerosol, the effect of atmospheric turbulence on the diffusion process of concentration bubble is explored in this section. Fig. 3 shows the diffusion of aerosol bubble in turbulent flow (initial is the same as Fig. 2). It can be seen that the atmospheric turbulence enhances the diffusion velocity of aerosol largely. Compared with Fig. 2, the maximum mass concentration drops to below $10 \mu g/m^3$ within 10 minutes under turbulence, and the spread range is much larger than that of calm atmosphere.

![Diffusion process under turbulent flow](image)

Figure 3. Aerosol diffusion process under turbulent flow.

(Inset: The vortex obtained by the vortex identification method of Liu et al. The atmospheric turbulence is generated by random initial potential temperature bubbles, and the...
maximum potential temperature perturbation is $PT_{pec} = 4.0K$.

### 3.2 Removal efficiency of wet scavenging under open air

In this section, the wet scavenging process is performed through introducing water drops to the local air, which is equivalent as water spray process. At initial, water spray is started at the center domain with a volume of $20 \times 20 \times 10m$ (central coordinates $x = 50m$, $y = 50m$ and $z = 50$). The release rate of water is $0.1 \text{kg} / (m^3 \cdot h)$, and the evaporation of water drops and condensation of vapors are also considered. Pollution is full of the whole domain and the mass concentration is $500 \mu g / m^3$. It is assumed that pollution decreases with a rate of $q_c = 30 \mu g / (m^3 \cdot \text{min})$ in the water spray domain, and the eliminate efficiency will be evaluated in the open air.
Fig. 4 shows the color map of the mass concentration after 5 minutes of wet scavenging. Seen from this figure, under the actions of convection and diffusion, the purified air spreads around rapidly and forms a relative larger purification domain. However, the purification domain is mainly located at a lower position due to the decrement of air temperature (evaporation of water drops absorbing heat) and increment of vapors. The turbulence enlarge the purification domain, while decreases the local efficiency to a certain extent. For example, the maximum mass concentration of aerosol are respectively \(371 \mu g/m^3\) and \(204 \mu g/m^3\) at \(t=5\) min.

As to the entire elimination efficiency, it can be seen from Fig. 5 that the total mass of aerosol in the water spray domain decreases by about 50% after half an hour. And the turbulence will not affect the comprehensive effect profoundly, but increases the scavenging rate to a certain extent.

4. CONCLUSIONS

The diffusion features of aerosol under calm and turbulent atmosphere are investigated based on a mesoscale large eddy simulation model. It is found that the diffusion of aerosol in calm atmosphere is very slow, while convection plays a major role in the transportation of particle material. The diffusion velocity of single aerosol bubble decreases with time, and turbulence enhance the diffusion velocity of aerosol to a great extent.

To the wet scavenging of aerosol in open air, the detailed elimination
efficiency is studied through introducing water drops to the local air. The results indicate that wet scavenging generally purifies the air near ground in open air, and the purification domain basically much larger than that of the water spray domain. Turbulence can enhance the purification domain, but the local elimination efficiency becomes worse. With a purification rate of $q_e = 30 \mu g/(m^3 \cdot \text{min})$, the total mass decreases by 50% within 30 minutes.

REFERENCES


