Simulation investigation of effect on nanoparticles discharging pattern of a car caused by a following one on a typical city road

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Abstract. Vehicle emission is supposed to contribute a great part to the urban air pollution in China, and many relative studies were carried out on a macro base at “city valley” scale. This article, on the “micro” individual scale otherwise, attempts to explore the fine particles’ spreading process after leaving the tailpipe of a typical car equipped with the inner-combustion engine in city main road through 3D CFD simulation. Two geometries of typical cars driving in typical city road were built up with detailed structures: one is one car driving on the main city street and the other is two cars, one followed the former established car, all with a driving speed of 40 km/h. Eulerian multiphase model is adopted to describe the dynamics of the multiphase: air, particles in 10nm diameter, and particles in 70nm diameter. The simulation results show that the diffusion process of 70nm particles is mainly governed by gravity, more than 80% of which concentrate within the region behind the car with a volume of 4.0m in length, 3.0m in height, and 2.0m in horizontal width along the centreline of tailpipe, while the 10nm particles exhibit a wider and more random distribution pattern, it spreads throughout the simulation volume with noticeable volume fraction: above, beneath, and behind the driving car, the high volume fraction regions mostly occur within a volume of 12.0m in length, 4.0m in height, and 4.0m in width associated with the tailpipe. The followed car causes a “compressing and lifting” effect, it is found that the high-volume fraction regions of particles are compressed to, on one hand, move around to the bodies of the two cars, and the other hand move towards the sides of the road. The particles in 70nm diameter are less affected by the followed car than that 10nm, especially the lifting effect of high-volume fraction regions of 10nm particles. This suggests some nonconventional management measures should be taken to control the urban air pollution of vehicles.

1. Introduction
As fog and haze weather conditions gradually prevailed most of the big cities throughout China in recent years, more and more attention has been paid to air pollution and the sources of pollution. Among many of them, vehicles with internal combustion engines streaming along city roads are supposed to be the major contributor, especially as a producer of microparticles pollutant [1], and many research has been conducted to explore the impacts of exhaust gas from internal combustion vehicles on the urban environment as the theoretical foundation for better air pollution controlling policies, such as Wang Jiasong [2], Ning zhi [3] and Fu Juan [4] investigated the distribution pattern...
of emission from a single car and the diffusion of particles and gaseous pollutants near the vehicle’s exhaust pipe, and Wang Yuancheng [5], You Xueyi [6], Wang Jiwu [7], and Ma Yintao [8] studied the distribution pattern of emission stream, the diffusion process of particle and gaseous pollutants in urban “street canyon”. Those studies above discovered the characteristics and diffusion process of emission pollutants discharging from internal combustion vehicles on roads in different scales.

As for the motor vehicles concerned above, schematic models, some of them were scaled-down, were applied to the moving vehicles on roads, and the vehicles were mostly simplified as line or surface pollution sources (non-point pollution source) and the emission factor was used to calculate the pollutant emission of vehicles [9,10,11].

To the particles involved, Jamriska M. [12] simulated the diffusion process of gaseous pollutants, mainly NOx and CO2 in a city canyon, and large-scale dimension, named as city canyon or valley, and it was the most adopted scenario in researches which includes a segment of street and all the vehicles on it. And the most investigated cases related particles were internal combustion engine industry, in which the diameter distribution of discharged particles was measured directly at the end of engine’s/vehicle’s tailpipes [13,14,15,16,17], the pollution pattern of particles from vehicles/vehicle under the city canyon scale was seldom investigated except for Jamriska [18] and Uhrner [19], they conducted a numerical simulation study on the particle emission from a light diesel truck.

From the point of view of air pollution management and control, it is suggested that the detailed structure and moving condition of vehicles should be taken into consideration, Hao Feilin [20] carried out a simulation investigation on the fine particles dispersion pattern after discharging from the tailpipe for a moving car with full detailed geometry, which took a step towards to the accurate and real simulation but did not consider the effect of following vehicles, in this research, a following vehicle was taken into account under a full scale, typical road setting, to explore the fine particles’ movement and diffusion process after its leaving the tailpipe, this may provide a better understanding of an early air pollution control for city.

2. Theory
The emission fume discharged from internal combustion engine vehicle is a mixture of gaseous and particle pollutants mainly composed of C, H, N, O and S, and could be described as multi-component, two-phase fluid in fluid dynamics, it could be set up either as a continuous fluid-based mixture governing by the Eulerian-Eulerian Multiphase Mode, or particle specialized flow as the Particle Transport (Lagrangian Particle Tracking) Model [21]. As the above research found, the particles in the vehicle’s emission characterized by relative lightweight for its carbon component with diameter of micron class, so its movement was largely affected by the gaseous flow, and continuous based Inhomogeneous Model of Eulerian-Eulerian Multiphase Model was the most suitable governing equation, which was developed from Navier-Stokes equation of single-phase flow by adding the interphase action, including momentum equation, continuous equation, volume conservation, pressure constraint and total energy equation [21] as followed.

Momentum equations:

$$\frac{\partial}{\partial t}(r_\alpha \rho_\alpha U_\alpha) + \nabla \cdot (r_\alpha (\rho_\alpha U_\alpha \otimes U_\alpha)) = -r_\alpha \nabla p_\alpha + \nabla \left( r_\alpha \mu_\alpha \left( \nabla U_\alpha + (\nabla U_\alpha)^T \right) \right) + \sum_{\beta=1}^{N_p} \left( \Gamma_{\alpha\beta}^* U_\beta - \Gamma_{\beta\alpha}^* U_\alpha \right) + S_{\alpha\alpha} + M_\alpha \tag{1}$$

Where: $\alpha, \beta$—describes the different phases of fluids in lowercase; $r_\alpha$—the volume fraction of phase $\alpha$; $\rho_\alpha$—the density of phase $\alpha$, kg/m³; $U_\alpha$—the velocity vector of phase $\alpha$, m/s; $\nabla$—the Hamilton operator; $\otimes$—the vector production operation; $p_\alpha$—the static pressure of phase $\alpha$, Pa; $\mu_\alpha$—the molecular (dynamic) viscosity of phase $\alpha$, Pa•s; $N_p$—the number of phases; $\Gamma_{\alpha\beta}^*$—represents the momentum transfer induced by interphase mass transfer; $\Gamma$—divergence operator; $S_{\alpha\alpha}$—momentum sources due to
external body forces, and user-defined momentum sources; \( M_\alpha \)—the interfacial forces acting on phase \( \alpha \) due to the presence of other phases.

Continuity equations:
\[
\frac{\partial}{\partial t} \left(r_\alpha \rho_\alpha \right) + \nabla \cdot \left(r_\alpha \rho_\alpha \mathbf{U}_\alpha \right) = S_{MSa} + \sum_{\beta=1}^{Np} \Gamma_{\alpha\beta}
\]

Where: \( S_{MSa} \)—user specified mass sources; \( \Gamma_{\alpha\beta} \)—the mass flow rate from phase \( \beta \) to phase \( \alpha \), kg/m\(^3\)*s; \n
Volume conservation equation:
\[
\sum_{\alpha=1}^{Np} r_\alpha = 1
\]

Pressure constraint:
\[
p_\alpha = p \quad \left( \alpha = 1, \ldots, Np \right)
\]

Total energy equation:
\[
\frac{\partial}{\partial t} \left(r_\alpha \rho_\alpha e_\alpha \right) + \nabla \cdot \left(r_\alpha \rho_\alpha \mathbf{U}_\alpha e_\alpha \right) = \nabla \cdot \left(r_\alpha \lambda_a \mathbf{T}_a \right) + r_\alpha \tau_a : \nabla \mathbf{U}_a + S_{sa} + Q_a + \sum_{\beta=1}^{Np} \left( \Gamma_{\alpha\beta} e_{\beta s} - \Gamma_{\beta\alpha} e_{\alpha s} \right)
\]

Where: \( e_\alpha \)—the internal energy of phase \( \alpha \), J; \( \lambda_a \)—the thermal conductivity of phase \( \alpha \), W/m*K; \( \tau_a \)—the shear stress of phase \( \alpha \), Pa; \( S_{sa} \)—internal heat source; \( Q_a \)—the heat flow rate to phase \( \alpha \), W/s; \( \left( \Gamma_{\alpha\beta} e_{\beta s} - \Gamma_{\beta\alpha} e_{\alpha s} \right) \)—describes the heat flow rate to phase \( \alpha \) from other phases due to mass transportation, W/s.

The particles discharged from vehicle with internal combustion engine was mainly composed of carbon and carbon oxides, when they (assuming them all spherical particles, denoted in \( \beta \) subscribe) dispersed into the continuous gaseous flow field (denoted in \( \alpha \) subscribe), would be acted upon by the continuous fluid, this could be described as follows.

\[
M_{\alpha\beta} = M_{\alpha\beta}^D + M_{\alpha\beta}^L + M_{\alpha\beta}^{LUB} + M_{\alpha\beta}^{VM} + M_{\alpha\beta}^{TD} + M_{\alpha\beta}^S + \cdots
\]

Where: \( M_{\alpha\beta} \)—the total interfacial force; \( M_{\alpha\beta}^D \)—the drag force; \( M_{\alpha\beta}^L \)—the lift force; \( M_{\alpha\beta}^{LUB} \)—the wall lubrication force; \( M_{\alpha\beta}^{VM} \)—the virtual mass force; \( M_{\alpha\beta}^{TD} \)—the turbulence dispersion force; \( M_{\alpha\beta}^S \)—the inter-particle collision force.

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\[
V_z = V_{10} \left( \frac{z}{z_{10}} \right)^{coe}
\]

Where: \( V_z \)—the wind speed of \( z \) (m) height from the ground, m/s; \( V_{10} \)—the wind speed of 10m height, m/s; \( z_{10} \)—reference height of wind speed, 10m; \( coe \)—ground characteristic coefficient, 0.1 for city street.

The influence of the ambient environment, especially the wind, on the flow field of vehicle emission is great, an exponential formula was included to simulation the ambient wind boundary condition.
investigation, seven kinds of particles in diameter was configured to simulate the emission of vehicle, they were: 10 nm, 70 nm, 100 nm, 300 nm, 500 nm, 1.0 mm and 2.5 mm, the percentage of each kind of particle was calculated by the literature above and field test measure (for particles larger than 100 nm), the particle emission rate of the vehicle was figured out by the engine displacement, engine speed and exhaust pipe diameter, which was verified later by the field test. During the simulation, all change in particle diameter induced by agglomeration, condensation, and reaction between particles when it moved among the gaseous flow after leaving the exhaust pipe.

3. Simulation setup
In this simulation scenario, a simplified geometry of car is constructed while driving on a typical city main street, in which a one-way city street with four lanes of 17.5m in width is set up including walkways illustrated in Figure 1. A Kia motor car (1.6L K3 of 2013) was selected for this investigation, and the corresponding simulation geometry is built according to the real body dimensions of K3, which is 4630mm (L)*1780mm (W)*1445mm (H), fitted with tires of 195/65 R15, the wheelbase and wheel-center-distance are 2700mm and 1555(F)/1568(R)mm respectively, the tailpipe is beside the inner side of the right rear wheel (a different simulation was verified with field test in literature [20]). The simulation boundary on the left in figure 1(b) was set as the green belt of road (1.5m height) center and the right as city buildings, the simulation boundary behind and front of the vehicle were set with a distance more than five times of the length of the vehicle, while a top simulation boundary is eight times from the top of the vehicle, then the simulation boundary in both sides figured out was more than three times from the vehicle as depicted in Figure 1. The following car exhibits the same geometry and driving speed, with a distance of 9.5m from the front car(two car body’s length).

![Figure 1. The car’s geometry for simulation.](image)
(a) side view of two cars  (b) back view  (c) side view of one car.

An unstructured tetrahedral mesh(Figure 2) was used to build the simulation volume with a dense grid of 50mm maximum length around the vehicle body, especially around the wheels and tailpipe, further control surfaces of the grid were set near the vehicle body and 500mm maximum length of grid was set in the area far from the vehicle body. About 2.67 million grid volumes were allocated for the simulation space, the quality index was 87%, 90% and 100% of Orthog. Angle, Exp. Factor and Aspect Ration respectively for the grid volumes, some other settings for the simulation was listed in Table 1.
Table 1. Some initial conditions, parameters and settings of simulation.

| Items                              | Value or setting                                                                 |
|------------------------------------|----------------------------------------------------------------------------------|
| Driving parameters of vehicle      | 11.11 m/s (40 km/h); 1.6L V discharging standard (GB18352.3)                    |
| Ambient                            | Ø50 mm (discharging pipe), 306.85 K; 1600 rpm (engine speed)                      |
| Gas/solid pair coupling model      | Interphase transfer: Particle Model; Drag force: Gidaspow Model                  |
|                                    | Lift force: Saffman Mei Model; Virtual mass force: Coefficient 0.5               |
|                                    | Wall lubrication: Antal Model; Turbulent dispersion force: Favre Averaged        |
|                                    | Turbulent transfer: Satio Enhanced Eddy Viscosity Model                          |
| Buoyancy model                     | Density Difference Model                                                         |
| Turbulence model                   | Gas phase: K-epsilon standard; Solid phase: Dispersed Phase Zero equation Model; Solid pressure model: Gidaspow Model |
| Turbulence initial                 | Medium Intensity and Eddy Viscosity Ratio                                        |
| Wall model                         | Free-slip Model                                                                  |
| Solving method                     | Finite volume method, fully implicit multi-grid coupled solution                  |
| Solving scheme                     | High resolution, double precision                                                 |
| Convergence iteration              | RMS, 0.0001                                                                      |
| Iteration parameters              | Step: 2s/10s, number of steps: 300                                               |

*a* Ansys, 2003.

4. Results and discussion

The simulation was carried out under some typical and ideal settings to simplifying the problem: 1) particles of 10nm and 70nm in diameters are selected to represent the tailpipe particles, for these two particles are the most parts of the gasoline engine[15,16,17]; 2) particles’ distribution is simulated from the tailpipe to the ground, resuspension of particles from solid surfaces and agglomeration due to particles collision are not concerned in the simulation, although they are a very significant phenomena in the air pollution research; 3) background pollution is neglected for particles’ collision is not simulated. Based on the above assumption, some of the results are visualized as figure 3-5. Figure 3 details the volume fraction contour of 10 nm and 70 nm particles, it stands for the volume proportion of specified particle to the surrounding atmosphere. Data was depicted on a vertical plane and a
horizontal plane, the vertical plane is the vertical plane section passing through the centerline of the tailpipe of the model car, while the horizontal plane is the horizontal plane section passing through the centerline of the tailpipe. For a better comparison, a grid was added in the figures as a dimension scale, the spacing between the horizontal lines is 1m while 2m for the vertical lines.

![Figure 3. Volume fraction contour of specified particles.](image)

![Figure 4. Comparison of averaged volume fraction of 10 nm particle on 5 vertical planes.](image)

![Figure 5. Comparison of averaged volume fraction of 70 nm particle on 5 vertical planes.](image)

Both 10 nm and 70 nm particles are in a very small volume fraction with orders of magnitude less than $10^{-7}$, so logarithmic coloring method was adopted for a clear contrast view. Particle with 10 nm diameter exhibits a more chaos distribution pattern, not only more widely spread in space but also in higher volume fraction, with a magnitude of more than $10^2$ times than that the 70 nm case, it suggests that the particle of 10 nm diameter constructs the major part of the particle pollution and be difficult to treat.

Figure 3(a) and (b) is a volume fraction comparison of 10 nm particle in the vertical plane between one car(a) and two cars(b), in both cases, particles propagate the whole studied volume that means persistent and wide-range pollution will be brought about. In the case of one car, higher concentration isolated areas of 10 nm particles stays in a spatial scope below 2m in height, while a more uneven distribution was found in the two cars case, higher concentration areas of particles move around the spaces within 4m behind the front car and over the following car, it could be inferred that the existence of the following car altered the pressure field between the two cars and produces a “press and split” effect, which pressing the particles to concentrate around the front and the follow-up, lifting them to a higher and wider space (>2m) while maintain the original particles below 1m. For the horizontal plane depicted in Figure 3(c) and 3(d), particles diffuse throughout the plane and random particle distribution could be observed, which spreads approximately in symmetric pattern alone the tailpipe in the case of one car, the follow-up car disturbs the random distribution by pushing the particles to gather around the two cars, while a diffusion of high concentration clusters of particle toward the two
sides, the center and the offside(pavement) of the road could be found, this suggests that green belts on the side and center of the road could play a more important role in particle pollution abatement.

In contrast to the particles of 10 nm diameter, sedimentation plays the leading role in the 70nm case. Figure 3(e)–(h) exhibits a better regular pattern of 70nm particles. It distributed mostly in the area behind the front car, within 4m behind the front car in the vertical plane and 2m symmetric along the tailpipe in the horizontal plane, almost all the exhausted particles spread under 1.5m in height. When the following car exists, it presses the 70nm particles towards around the front car and confines the containments in a smaller area, which suggests a smaller impact on the environment and be easier for management.

Figure 4 shows the averaged volume fraction of 10nm particles in 7 selected parallel vertical planes perpendicular to the centerline of the tailpipe, the abscissa is the distance in meters from the tailpipe end. It could be observed that a sedimentation of particles both 10nm and 70 nm considerably takes place in the one car case, a decrease of more than 80% in 70nm particle’s volume fraction could be calculated within 2m distance due to the sedimentation process, while in the 10nm case, a decrease of less than 50% is obtained with sedimentation through 12m distance. When there is a car followed, it causes significant effect for the 10nm particles, an increase in volume fraction occurs especially around the follow-up car, this could be brought about for a disturbance of the particles behind the front car area which causing the supposed settled particles re-entering the atmosphere, in the region near the follow-up car, disturbance and self-producing particles together cause an averaged volume fraction increase of nearly 2 times as that the one car case. Figure 5 illustrates the comparison of 70nm particles volume fraction in 7 selected planes, a dramatic decrease in volume fraction with distance could be observed and the following car has an insignificant effect on the front car.

5. Conclusions
In this paper, an ideal and simplified configuration of road and cars is preliminary explored and simulated, particles of 10nm and 70nm diameters are selected as the representative of exhausting particles of gasoline engine vehicles, some conclusion could be drawn from the simulation as follows:

The particles exhausting from a vehicle are characterized by a backward and downward diffusion because of gravity and forward-running of the car, in this process particle size plays a significant role in the diffusion pattern, particles of 70nm diameter mostly distributed within a spatial scope behind the car, with a typical dimension3 in this article is 4.0m in length, 3.0m in height, and 2.0m in horizontal width along the centerline of tailpipe. As a contrast, the particles in 10nm diameter spread through the whole volume simulated with higher concentration clusters be similar to the 70nm ones, but with a wider extends: 12.0m in length, 4.0m in height, and 4.0m in width, this suggests that it is more difficult to handle the 10nm nano-particle air pollution.

When the car is followed by another car in this investigation, a “compressing and lifting” effect is caused, which would compress the particles to spread towards the bodies of the two cars while widening its spread scope in height and width. It is dramatic for 10nm particles high concentration regions propagate toward higher, wider spatial scope, but for the particles of 70nm diameter this effect become insignificant, a decrease of more than 80% in volume fraction could be attained within 2.0m distance behind the car due to gravity sedimentation in contrast to less than 50% through 12m distance for 10nm particles.

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