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Sensitivity analyses of ultrafine particle dispersion inside an isolated street canyon

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ABSTRACT

Ultrafine particles originating from vehicle exhausts may deteriorate the air quality inside the street canyon, so it is of importance for the air quality control to clarify the formation and dispersion characteristics of ultrafine particles. In this study, the population balance model considering the nucleation, condensation and evaporation, as well as the species transport and RNG k-ε turbulent models were employed, and the sensitivities of the dispersion of ultrafine particles to the wind direction, emission rates of H_2SO_4 vapor and organic compounds, traffic flow and ambient temperature inside an isolated street canyon were analyzed. The results show that the wind direction is a key issue to the particle number concentration. The emission rates of H_2SO_4 vapor and organic compounds play dominant roles in the formation and growth of particles, so should be strictly controlled to reduce the air pollution. Restricting the use of private vehicles based on the even-and-odd number licensed trip can conspicuously lower the ultrafine particle concentrations by more than one order of magnitude. More powerful nucleation among the vehicle exhausts will be triggered in a cold environment, therefore the haze pollution may break out in winter more easily.

1. Introduction

The respirable ultrafine particles emitted from vehicles, which are the major sources of the particles in the urban environment [1], can pose a threat to human health and cause the diseases such as lung cancer [2], cardiovascular disease [3] and asthma [4] et al. The emitted plume from vehicles contains the precursor gases to form the nuclei by nucleation [5] and the soot mode particles generated from engine combustion. The diameters of these particles are usually smaller than 100 nm. For the nuclei with the size <10 nm, the compositions are mainly some molecules of organic vapors. While the soot mode particles are basically composed of black carbon, nearly 80%, and some organic compounds. The pedestrians, shop vendors and residents near the street are more easily exposed to ultrafine particles than others [6]. Therefore, it is vital to investigate the transport characteristics of ultrafine particles near the street. Gromke et al. [7] investigated the influences of wind direction, aspect ratio of street on the dispersion of gas pollutants inside the street canyon by wind tunnel tests, concluding that the wind direction and aspect ratio primarily affect the pollutant concentrations inside the canyon. Besides, many numerical studies [8–15] were also made, including the impacts of solar radiation, the shape of the roofs on flanking buildings and the urban street layout et al.

The aforementioned works show that more emphases were placed on the impacts of ambient conditions and buildings upon the pollutant transport inside the canyon, the discussions about vehicles are seldom. In most studies, the vehicles are replaced by an equivalent line or point emitting source. However, the vehicle induced turbulence may play an important role in the transportation of the pollutants according to Wang and Zhang [16]. Furthermore, the nucleation, condensation and evaporation processes in the exhaust plume are often ignored, although they are commonly critical to accurately comprehend the dispersion characteristics [17–19]. In this work, the population balance model taking the nucleation, condensation and evaporation into account, as well as the species transport and RNG k-ε turbulent models were adopted to investigate the dispersion of ultrafine particles inside an isolated street canyon, in which the vehicle induced turbulence was also considered.

2. Mathematical model

2.1. Turbulent airflow transportation model

According to the work of Salim et al. [20], large eddy simulation is currently the best choice in capturing the characteristics of the turbulent air flow in street canyon. However, the computational cost is so expensive that limits its applications. As a balanced approach, the k-ε turbulent model, which can also be able to predict the main flow

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features and requires a relatively small computational cost, has increasingly been used in many simulations. In this study, the Reynolds averaged Navier-Stokes equations and energy equation combined with the Renormalization Group (RNG) k-ε model are adopted. The continuity, momentum and energy equations are given below:

$$\nabla\cdot\left(\rho\vec{v}\right)=0 \tag{1}$$

$$\nabla\cdot\left(\rho\vec{v}\vec{v}\right)=-\nabla p+\nabla\cdot\left(\bar{\bar{\tau}}\right)+\rho\vec{g} \tag{2}$$

$$\nabla\cdot\left(\vec{v}(\rho E+p)\right)=\nabla\cdot\left(k_{\mathrm{eff}}\nabla T-\sum_j h_j\vec{j_j}+\left(\bar{\bar{\tau}}\cdot\vec{v}\right)\right) \tag{3}$$

where $\vec{v}$ is the time average velocity. p is the mean pressure, ρ is the density and $\bar{\bar{\tau}}$ is the stress tensor and $\rho\vec{g}$ is the gravitational force. In Eq. (3), $E = h\text{-}p/\rho + v^2/2$, h is the sensible enthalpy, k_{eff} is the effective conductivity, $\vec{j_j}$ is the diffusion flux of species j. The fluctuations associated with turbulence have impacts on the time-averaged Navier-Stokes equations, where the velocity fluctuations produce additional stresses in the fluid, the so-called Reynolds stresses, which need to be modeled to mathematically close the problem. The transport equations for k and ε in the RNG k-ε model take the following forms:

$$\nabla\cdot\left(\rho k\vec{v}\right)=\nabla\cdot\left(\alpha_k\mu_{\mathrm{eff}}\nabla k\right)+G_k+G_b-\rho\varepsilon \tag{4}$$

$$\nabla\cdot\left(\rho\varepsilon\vec{v}\right)=\nabla\cdot\left(\alpha_k\mu_{\mathrm{eff}}\nabla\varepsilon\right)+C_{1\varepsilon}\frac{\varepsilon}{k}\left(G_k+C_{3\varepsilon}G_b\right)-C_{2\varepsilon}\rho\frac{\varepsilon^2}{k}-R_\varepsilon \tag{5}$$

where k is the turbulent kinetic energy, ε is the turbulent dissipation rate, μ_{eff} is the effective viscosity, α_k and α_ε are the inverse effective Prandtl numbers for k and ε, G_k and G_b represent the generations of turbulence kinetic energy due to the mean velocity gradient and due to buoyancy. The term of R_ε originates from the effects of rapid strain and streamline curvature. The coefficients are $C_{1\varepsilon} = 1.42$, $C_{2\varepsilon} = 1.68$ [21].

A commercial CFD software FLUENT is applied to solve the equations mentioned above in the form of discretized algebraic equations with a second-order upwind scheme. The SIMPLE algorithm [21] is employed to couple the pressure and velocity fields. In addition, the temperature distribution in the street canyon may affect the pollutant dispersion process [8], so the Boussinesq approximation is used.

2.2. Species diffusion model

Gas pollutants like H_2SO_4 vapor and many organic compounds will disperse in the canyon after emission from the vehicle tailpipe. The species diffusion equation is expressed as follows [21]:

$$\nabla\cdot\left(\rho\vec{v}Y_i\right)=-\nabla\cdot\vec{J_i}+S_i \tag{6}$$

$$J_i=-\left(\rho D_i+\frac{\mu_t}{Sc_t}\right)\nabla Y_i \tag{7}$$

where J_i represents the mass diffusion of gas pollutants, S_i is the source term equal to the mass transfer between the gas and particles, D_i is the molecular diffusion coefficient for the pollutant in the mixture, $\mu_t = \rho(C_\mu k^2/\varepsilon)$ is the turbulent viscosity, Y_i represents the mass fraction of pollutants and ρ is the mixture density. $Sc_t = \mu_t/(\rho D_t)$ is the turbulent Schmidt number, where D_t is the turbulent diffusivity. In this study, Sc_t is set as the typical value of 0.7 [7].

2.3. Particle dispersion model

Vehicles running in the street canyon can directly eject soot mode aerosol particles originating from the engine combustion. Moreover, the gas exhausts containing H_2SO_4 vapor and organic species can also form nano-scale particles by the process of nucleation [22]. The soot mode and nucleated new particles will grow or shrink due to the condensation, evaporation and coagulation processes. The transport of the microscale or nanoscale aerosol particles related to the vehicles is governed by the Population Balance Equation (PBE) [23], which can be expressed as:

$$\underbrace{\nabla\cdot\left[\vec{v}n\left(V,\vec{x},t\right)\right]}_{\text{Advection term}}+\underbrace{\nabla_V\cdot\left[G_V n\left(V,\vec{x},t\right)\right]}_{\text{Growth term}}=$$
$$\underbrace{\frac{1}{2}\int_0^V a\left(V-V',V'\right)n\left(V-V',\vec{x},t\right)n\left(V',\vec{x},t\right)dV'}_{\text{Birth due to Coagulation}} \tag{8}$$
$$\underbrace{-\int_0^\infty a\left(V,V'\right)n\left(V,\vec{x},t\right)n\left(V',\vec{x},t\right)dV'}_{\text{Death due to Coagulation}}$$

where n is the particle size distribution (PSD) function, which depends on the particle volume V, coordinate vector $\vec{x}$ and time t; G_V is the growth rate based on the particle volume. The right hand side of the equation is the coagulation terms in which a represents the coagulation

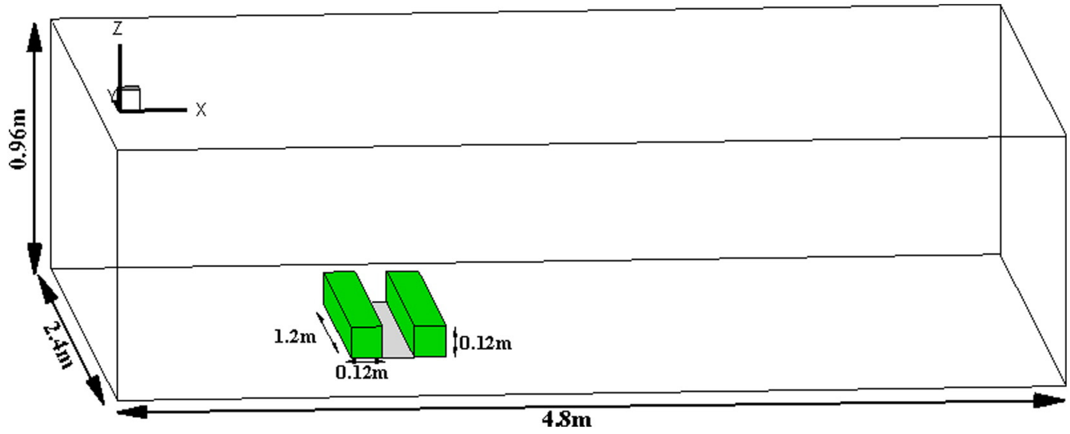

Fig. 1. Computational domain for the validation experiment.

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