



Direct quadrature method of moments for the exhaust particle formation and evolution in the wake of the studied ground vehicle

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ABSTRACT

In the present study, the particle formation and evolution processes, and concentration field in the wake region of the studied ground vehicle for stationary (i.e., low idling mode) and moving (i.e., 10 and 30 km/h modes) conditions in a typical high densely urban road microenvironment were investigated numerically using large eddy simulation (LES) with the aerosol dynamics and dispersion model based on the direct quadrature method of moments (DQMOM) approach. The turbulent dilution and dispersion characteristics, and the complex formation and growth dynamics of exhaust particles behind the studied ground vehicle to the atmosphere were taken into consideration. The results show that the processes of nucleation and coagulation are completed in a short distance away from the vehicular exhaust tailpipe exit of the studied ground vehicle. Due to the nucleation, coagulation and strong dilution by the turbulent exhaust plume that take place behind the studied ground vehicle, the characteristics and behavior of the average diameter, and the number and volume concentration of the particles are quite different with respect to the studied driving conditions.

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1. Introduction

Motor vehicles are the major source of air pollutants in most densely populated urban cities. Many chronic and acute effects on human health/carcinogen have been known clearly to be associated with personal exposure to the range of nano- ($D_p < 0.05 \mu\text{m}$ or 50 nm) to fine ($D_p < 2.5 \mu\text{m}$) particles in the recent health and epidemiological studies (Davidson, Phalen, & Solomon, 2005; Morawska, Moore, & Ristovski, 2004; Penttinen et al., 2001; Pope & Dockery, 2006; Sioutas, Delfino, & Singh, 2005; Stone & Donaldson, 1998). The particle size mainly concentrates on nanometer to micrometer due to unburned fuel and lubricating oil, sulfate, exhaust cooling and particles aggregation (Jacobson, Kittelson, & Watts, 2005; Kittelson, 1998; Wong, Chan, & Leung, 2003). The typical usage of sulfur content in diesel fuels for the developed and developing countries ranged from 10 to 2000 ppm S. When the combustion of diesel fuel takes place inside the engine, most of the sulfur transforms into sulfur dioxide (SO_2) and a small part can be directly oxidized into sulfuric trioxide (SO_3). If the diesel particle filter is taken into consideration, the conversion rate can then be higher (Uhrner et al., 2007). Because of the abundance of water vapor in the exhaust gas, SO_3 can be transformed into sulfuric acid (H_2SO_4) easily and then form new particles due to nucleation effect. This transformation can be characterized by the parameterization of the sulfuric acid-water vapor binary system (Kulmala, Laaksonen, & Pirjola, 1998; Vehkamäki et al. 2002; Vehkamäki, Kulmala,

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Lehtinen, & Noppel, 2003). It clearly indicates that sulfuric acid may contribute to serious environmental problems and be harmful to people's health. Hence, it is of great importance to have a better understanding of the formation and evolution processes of vehicular exhaust particles in the wake region of the studied ground vehicles for different driving conditions in urban road microenvironment. Zhang and Wexler (2004) investigated the exhaust pollutants from on-road vehicles into two stages namely, tailpipe-to-road and road-to-ambient conditions. The former stage takes place in the first 1–3 seconds, while the latter stage often takes place in the last 3–10 minutes. The particle distribution from the vehicular exhaust jet plume in the near-field is important to be quantified because the eventual redistribution of particle in the far-wake region is highly dependent upon the particles formed from the vehicular exhaust jet plume in the near-field. In the present study, major attention will be paid to the first stage (i.e., tailpipe-to-road condition). However, such formation and evolution of the vehicular exhaust particles is a very complex process involving nucleation, dispersion, coagulation and surface growth in respect to different characteristic time. Generally speaking, nucleation has a much smaller characteristic time than the other processes. Recently, Upadhyay and Ezekoye (2005) have stated that the nucleation process takes place much faster than coagulation process while Prakash, Bapat, and Zachariah (2003) have showed that the characteristic time of nucleation is about 10^{-7} to 10^{-8} second. This incompatibility in characteristic time-scale will lead the numerical simulation to a dilemma because such time-scale in nanosecond is too small for most engineering applications.

With more powerful computers and advanced numerical techniques, it becomes possible to investigate the flow and dispersion characteristics, and formation and evolution processes of vehicular exhaust particles in the wake region of the studied ground vehicle for different driving conditions in urban road microenvironments using large eddy simulation (LES) with the aerosol dynamics and dispersion model based on the direct quadrature method of moments (DQMOM). However, only limited studies have been done in the particle flow with sulfuric acid (Lemmetty et al., 2006; Pohjola, Pirjola, Kukkonen, & Kulmala, 2003, 2006). In the present study, the particle flow around a driven ground vehicle will be studied. The particles are first generated from nucleation (i.e., sulfuric acid-water vapor binary system) and then coagulated with each other. There are two problems i.e., flow structures development, and the particles formation and evolution concerned during the simulation. Since the particles are too small (i.e., around nano-meter magnitude and Stokes number $St \ll 1$), the particles follow the gas flow streamline perfectly. It is reasonable to consider the flow and the particle fields separately, and neglect the influence of particles on the gas flow.

Richards, Wright, Baker, and Baxendale (2000) used the k - ϵ , RNG k - ϵ and k - ϵ /Chen turbulence models to study the pollutant dispersion in the near-wake region of vehicles. Chan and Dong (2001) studied the initial dispersion process of NO_x , temperature and flow structure from a vehicular exhaust plume using the joint-scalar probability density function approach coupled with a k - ϵ turbulence model. Kim, Gautam, and Gera (2001) also developed a three-dimensional numerical model coupled with k - ϵ model to study the dispersion of carbon dioxide (CO_2) from a heavy-duty truck exhaust plume. Jiang et al. (2005) studied the evolution of particle size distributions in vehicle exhaust plumes with unconfined dilution by ambient air using the computational fluid dynamics (CFD) with an aerosol dynamics model. Recently, Roy, Payne, and McWherter-Payne (2006) have investigated numerically the flow structure, drag force and pressure distribution of a simplified tractor/trailer geometry using the Reynolds-averaged Navier-Stokes (RANS) simulation. Although k - ϵ or RNG k - ϵ model is often adopted to calculate the flow field in engineering application, it is always denounced for its accuracy in complex turbulent flow. In addition, the RANS equations are a time-averaged numerical method, so they cannot capture the flow and the species in respect to time. On the contrary, the LES takes the space average of a variable, so it can describe the flow and the species instantaneously. Recently LES approach has been used to calculate the flow structures and pollutant dispersion behind the studied ground vehicle (Chan, Luo, Cheung, & Chan, 2008a; Chan et al., 2008b; Dong & Chan, 2006; Yin, Lin, Zhou, & Chan, 2007; Yin, Lin, & Zhou, 2008).

The evolution of nano-particles is controlled by the general dynamic equation (GDE) (Friedlander 2000), which is a nonlinear, partial differential equation (Talukdar & Swihart, 2004). Although the GDE is capable to describe the evolution of particles under all kinds of influence (e.g., convection, diffusion, coagulation, nucleation, surface growth and other physical or chemical phenomena), it is difficult to be solved mainly because of its dependence on particle volume, v . As a compromise, several numerical techniques have been developed to cover this shortcoming. Among these methods, the sectional methods (Garrick, Lehtinen, & Zachariah, 2006; Miller & Garrick, 2004; Mukherjee, Prakash, & Zachariah, 2006; Settumba & Garrick, 2003) divide the particle volume space into several discrete sections or bins. At each section or bin, the particle volume is considered to be a constant and the GDE can be numerically solved much easily. Pohjola et al. 2003, 2006) utilized the sectional method to model the influence of aerosol process for the dispersion of vehicular exhaust in street environment. Another method is the method of moment (McGraw, Nemesure, & Schwartz, 1998; Settumba & Garrick, 2004). It takes the moments of particle size distribution (PSD) on the entire particle volume space. The GDE can be transformed into a set of moment equations (Diemer & Olson 2002). The closure problem arises because solving a finite number of moment equations requires the absent (usually high order) moments to evaluate the correlative term (Diemer & Olson, 2002). Again, some models have been introduced into the simulation in order to solve the closure problem. The classical moment of method usually takes some assumption to make the moment equations closed such as assuming the PSD is mono-dispersed (Kruis, Kusters, Pratsinis, & Scarlett, 1993) or log-normal distributed (Bensberg, Roth, Brink, & Lange, 1999). Uhrner et al. (2007) have recently studied the dilution and aerosol dynamics in a diesel car exhaust plume using the CFD codes and log-normal assumption. McGraw (1997) proposed a new method known as quadrature method of moment (QMOM) to make the moment equations closed. Based on the theory of McGraw (1997), Fox (2003) further developed a new method named direct quadrature method of moments (DQMOM), which has been proved to be

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