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Determining the relationship between chemical composition and size, shape and effective density of airborne fine particles through concurrent use of inertial and optical based measurements

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ABSTRACT

This study presents the development of a medium flow, multiple slit based $PM_{2.5}$ (particle aerodynamic diameter <2.5 μm) inertial impactor. Its performance was compared with that of a light scattering based optical particle sizer in a field study and in controlled lab based experiments using polydisperse dolomite powder as test aerosol. The impactor's optimum nozzle configuration had a cutoff size of 2.51 μm (aerodynamic diameter) at an operating flow rate of 215 L/min with a pressure drop of 0.35 kPa across the impactor stage. Because the apparent particle density of an ambient aerosol depends on the physical properties and the chemical composition of the particles, the $PM_{2.5}$ mass concentration was measured with an optical particle sizer and an inertial impactor over a weekday and a weekend day in a field study during which the effective particle shape factor and density were in tandem modified in order to compare the results from the two sampling techniques. The correlation of the two instrument results tended towards 1:1 with increasing values of shape factor (irregular shaped) and effective particle density. This observation was supported through chemical investigations of the collected mass, which showed a higher percentage contribution from elements which are mostly of crustal nature (namely, Ca, Fe, and Mg).

Introduction

Epidemiological and toxicological studies conducted in the past have conclusively shown that particulate matter (PM) causes adverse health effects in humans (Dockery et al., 1993; Harrison, Giorio, Beddows, & Dall'Osto, 2010; Koenig et al., 2005). Additionally, PM also affects climate, regional visibility, and the deposition of acidic and toxic substances. Numerous epidemiological studies (Korrick et al., 1998; Neas, Schwartz, & Dockery, 1999; Schwartz & Dockery, 1992) have shown an association between exposure to fine PM with aerodynamic diameters <2.5 μm ($PM_{2.5}$) in ambient air and increase in morbidity and mortality rates, adverse effects on respiratory function and cardiovascular dysfunctions. Studies have also shown a correlation between mass concentration of $PM_{2.5}$ and adverse health effects in at-risk populations (the elderly and ill) (Pope et al., 2002).

With increasing economic development, anthropogenic sources of aerosols have grown exponentially. Industry, domestic fuel burning, vehicular emissions, and other such sources contribute to ambient particulate matter concentration. The processes involved in generating particulate matter from these varied sources and their interactions with their surroundings affect and transform the particles' initial properties, such as their size, shape, and chemical composition. Many instruments have been developed to measure their number, mass, or chemical species concentration as a function of particle size (Baron, Mazumder, & Cheng, 2001; Flagan, 2001; Jayne et al., 2000; Wexler & Johnston, 2001).

Atmospheric particles often deviate from the characteristics of an ideal particle, i.e. spherical shape and standard density of 1.0 g/cm^3. For example, soot aggregates are non-spherical particles (Katrinak, Rez, Perkes, & Buseck, 1993), one of the major sources of which are diesel emissions. The shape factor of particles is near unity for particles which are near-spherical, while irregularly shaped particles have higher values. An important area of current aerosol research is the physical and chemical characterization of non-spherical and fractal particles (Park, Cao, Kittelson, & McMurry, 2003; Tammet, 1995). In addition to mass concentration,

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analysis of a particle's surface and its chemical composition is also relevant for toxicological and epidemiological studies (Bérubé et al., 1999; Gilmour et al., 1996). Particle deposition in the lungs by sedimentation and inertial processes is directly controlled by particle size, shape, and density. Knowing particle shape and density can improve model lung deposition calculation results.

When PM mass concentration and particle size are measured in parallel, density data can be obtained from the ratio of mass concentration and integrated volume concentration for the overlay size range of both instrumental setups. As a result, the error of this parameter includes errors from both setups. The density calculated in this study is an average density for all spherical particles up to an aerodynamic diameter of 2.5 μm, hence it is referred to as "apparent density", since it might be totally different from the bulk density of the particulate material as indexed in other studies. This is because average density depends on the physical and chemical composition of the particle populations sampled. For example, Park, Kittelson, Zachariah, and McMurry (2004) found that the density of diesel exhaust particles increased from 1.27 to 1.78 g/cm^3 as particle mobility size increased from 50 to 220 nm and that when particles were preheated to remove volatile components, the density was 1.77 ± 0.07 g/cm^3, independent of particle size. Particles from crustal erosion processes such as wind erosion or road dust events are expected to consist of dispersed bulk material which has undergone erosion and fracture mechanisms; such particles have a bulk density of about 2.7 g/cm^3 (Hänel & Thudium, 1977; Shur, Harris, Jones, Kaerger, & Price, 2008).

Particle density and shape are important aerosol properties that affect particle transport phenomena such as dry deposition and cloud scavenging. Furthermore, density and shape affect conversion calculations from particle size (or volume) to mass, which is an important parameter for particulate exposure and governmental regulation (Pope, 1996; Wichmann et al., 2000). This conversion is also used in the comparison of mass and number based sizing instruments such as multi-stage impactors, aerodynamic particle sizers (APS), differential mobility analyzers (DMA), scanning mobility particle sizers (SMPS), and tapered element oscillating microbalances (TEOM). Studies using a DMA-TEOM impactor (Pitz et al., 2003) and a SMPS-APS-TEOM impactor (Khlystov, Stanier, & Pandis, 2004) were conducted to determine the mean apparent particle density for $PM_{2.5}$. Further, a SMPS-TEOM setup was used to analyze the mean apparent particle density of submicron PM (Morawska, Johnson, Ristovski, & Agranovski, 1999). The role of particle shape and chemical composition in determining the apparent density was ignored in those and similar studies. However, there have been several studies reporting the PM composition either season wise or over weekday/weekend (Hassan, El-Abssawy, AbdEl-Maksoud, Abdou, & Khoder, 2013; Khoder & Hassan, 2008). Such studies give an insight into the role of the sources that contribute to the various chemical species of PM in the atmosphere. Therefore, we developed a medium flow slit based $PM_{2.5}$ inertial impactor and tested its performance in the lab. This study aims to further understand the effects of varying effective particle density and shape factor on $PM_{2.5}$ mass concentrations obtained from an optical particle sizer by comparing its measurements with those obtained using our novel impactor over a weekday and a weekend day.

Materials and methods

Description of the sampling instruments

Design, fabrication, and lab evaluation of a slit based, medium flow $PM_{2.5}$ impactor

Inertial impactors are quite simple devices in which air containing suspended particles flows around an impaction substrate and is subjected to a sharp change in its flow trajectory. Sharply bending air streamlines forces the particles with sufficient inertia to slip across the streamlines and impact on the impaction surface while finer particles (with lower relaxation time) will simply follow the bending air streamlines and move downstream of the impaction substrate (Hinds, 1999). In order to measure PM concentrations of different size bins, various inertial impactors have been developed over the years (Demokritou, Lee, Ferguson, & Koutrakis, 2004; Sioutas, Ferguson, Wolfson, Ozkaynak, & Koutrakis, 1997).

Since other low and high flow rate impactors have been developed at IIT Kanpur (Gupta, Chakraborty, & Ujinwal, 2010; Gupta, Jaiprakash, & Dubey, 2011; Kumar & Gupta, 2015), design considerations and methodology similar to those used in previous impactor designs, were adopted in developing this novel slit based impactor. The cutoff size of the impaction stage can be calculated by using the Stokes equation, which can be formulated as follows (Baron & Willeke, 2001; Hinds, 1999):

$$Stk = \frac{\rho_p d_p^2 U C_c}{9 \eta W}, \quad (1)$$

where ρ_p is the particle density (kg/m^3), η is the dynamic viscosity of air (Pa s), d_p is the particle diameter (m), U is the jet velocity in the impactor nozzle (m/s) given by the ratio of flow rate (Q) and area of cross-section of the nozzle (A), W is the nozzle width (m), and C_c is the Cunningham slip correction factor. The theoretical value of $\sqrt{Stk_{50}}$ was taken as 0.70 for the design of the slit nozzle (Marple & Liu, 1974; Marple & Willeke, 1976) ($\sqrt{Stk_{50}}$ is the value of $\sqrt{Stk}$ at 50% cutoff diameter). The nozzle Reynolds number (Re) was calculated using the following equation:

$$Re = \frac{2UW\rho_{air}}{\eta}, \quad (2)$$

where ρ_{air} is the air density (kg/m^3) and U is the flow velocity (m/s) at standard conditions (Hinds, 1999).

Various slit based impactor nozzles were designed for $PM_{2.5}$ based on Eq. (1). The impactor nozzles along with the impaction substrate unit were tested individually using a laboratory testing rig setup as shown in Fig. 1(b). An improved dry aerosol generator (the design of the dispersion nozzle was modified to improve the performance of an existing aerosol generator) was employed using dolomite powder to produce a stable flow of polydisperse aerosol (Gupta et al., 2011; Singh, Gupta, Tripathi, Jariwala, & Das, 2011). The shape and size of the dolomite powder particles used for generating the dry aerosol was analyzed using a scanning electron microscope. The results from the electron microscopy showed that these particles are partially bounded by rhombohedral planes and form an interconnected network (Kretz, 1988). This implies that in the absence of spherical polystyrene latex (PSL) particles, finer dolomite powder may be an acceptable option for a test aerosol. Because the finer dolomite particles have a compact shape that is close to being spherical it is fair to assume that the dynamic shape factor is 1.10; particle density is 2840 kg/m^3 (Alkuwairan, 2012; Deelman, 1999). The dolomite powder was sieved through a 45-μm mesh and the finer fraction was used as the test aerosol to avoid clogging the air inlets and nozzles in the aerosol dispersion chamber. The generated aerosol enters the mixing chamber where it is mixed and diluted with dried, high-efficiency particulate arrestance (HEPA) filtered ambient air to control particle loading on the substrate. Then the diluted aerosol enters into a cylindrical duct of approximately 2 m length on the upstream side of impactor assembly to ensure complete mixing and uniform concentration of aerosol at the sampling point. A high flow rate vacuum pump was employed to generate the desired flow rate. This flow rate was monitored by a rotameter previously calibrated with a mass flowmeter (Model 4040, TSI Inc., USA).