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Deposition efficiency of fractal-like aggregates in fibrous filters calculated using Brownian dynamics method

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Abstract

Nonspherical particles, such as fractal-like aggregates emitted by diesel engines, are commonly met in the ambient air. Some of them are believed to be carcinogenic to humans, thus their efficient removal is of crucial practical importance. A fibrous filter is the device commonly used for aerosol purification but the literature lacks experimental data concerning aggregates filtration. Effect of aggregates' parameters (fractal dimension, primary particle radius) as well as fiber diameter and air velocity on the filtration efficiency is investigated theoretically using the modified Brownian dynamics method. Three different expressions for the friction coefficient evaluation for the aggregates were examined. The results obtained indicate that structure of an aggregate, filter structure and process conditions strongly influence the aggregates deposition efficiency, which significantly differs from the values determined for mass-equivalent spherical particles. The results determined using the Brownian dynamics approach were compared with the values calculated using classical single fiber theory and noticeable discrepancy was observed for the most penetrating particles, while both approaches agree for the limiting cases of small or large particles. Peclet number based on the mobility radius and the interception parameter based on the outer radius are the proper criteria to describe diffusional and deterministic deposition of aggregates.

Keywords: Aerosol; Aggregate; Brownian dynamics; Cluster; Deposition; Fibrous filter; Filtration

1. Introduction

Spherical aerosol particles are usually used to assess a fibrous filters efficiency experimentally. This efficiency is commonly considered to be the same for all particles of the same size and density for a given filter and process conditions. However, a particle shape may significantly influence its deposition efficiency. The atmospheric air contains many nonspherical particulates, which might be filtered out with substantially different efficiency than that one evaluated during laboratory tests performed using spherical aerosol particles. Fractal-like aggregates are probably the most important kind of nonspherical particles that are commonly met in the air. They may be formed in various processes, e.g., combustion for power generation and pigment production, pharmaceutical drug delivery, and manufacture of carbon black or other materials [1,2]. The largest amount of atmospheric carbon black (or soot) particles is probably emitted by diesel engines [3]. The agglomerated diesel exhausts are particularly hazardous, since they can contribute to the development of lung cancer and may cause cardiovascular and acute and chronic noncancer adverse respiratory health effects [4–6]. Diesel exhaust has been classified as probably carcinogenic to humans [7]. In addition to the adverse human health effects, the emissions of the diesel engines contribute to the reduction of visibility, global climate change, soiling of buildings, substantial damage to the material exposed and reduction of ground water quality [4,5]. To limit the exposure to such aggregates, their efficient filtration is necessary, but to design an optimal filter structure for the aggregates' filtration, a precise knowledge on how the aggregate structural parameters influence their deposition efficiency is needed first. Minimization of agglomerated particulates will be a very challenging task for cars' manufacturers as legal regulations concerning engines exhaust purity become much stricter nowadays, and fibrous filtration is considered as a promising method to achieve this goal.

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The aggregates are composed of many fine particles (primary particles) attached together. The size of the primary particles is usually between 5 and 50 nm [8], while the whole aggregates have the sizes from about 100 nm to several micrometers [9]. The aggregates composed of fine particles are not fractals in strict sense of this word, since at small scales they contain nonfractal subunits They are fractals in such a sense that the cluster mass varies with its radius to a fractional power [10], thus they are called "fractal-like" aggregates. Fractal-like aggregates have self-similar structure, which means that they look the same under different magnifications. It is commonly assumed that really existing aggregates have average or statistical self-similarity, which indicates that the correlation functions describing the structure of fractal-like aggregates have a scale invariant (power law) form [11].

The structural parameters of the fractal-like aggregates (e.g., fractal dimension, radius of primary particle) may affect the filtration efficiency of the aggregates in fibrous filters. However, due to a complex structure of the clusters, and therefore difficulties in their reproducible generation, precise characterization of their structure and interpretation of the raw data obtained with aerosol counting instruments, the filtration of the aggregates is a subject of very little experimental studies and the experimental data are rare and not easy for interpretation. This makes a theoretical analysis of the process an attractive alternative that may provide many useful information, which are unavailable experimentally. Thus, the goal of our paper is to investigate theoretically effect of the fractal dimension, size of the primary particle, fiber radius, and gas velocity on the fractal-like aggregates' deposition efficiency onto a single fiber in a fibrous filter. The numerical simulations were performed using the modified Brownian dynamics method, while the mobility and the maximum (outer) aggregate radii were determined using the model proposed by Lattuada et al. [12,13], which is based on the Kirkwood–Riseman theory and Monte Carlo simulations. Various approaches recommended in the literature were used in order to obtain the values of the friction coefficient for the aggregates. Moreover, the results were compared with the data obtained from the commonly used classical single fiber theory.

2. Method

Deposition of aerosol particles onto a fiber in a filter can be caused by various mechanisms, such as: diffusional mechanism, interception, inertial impaction, gravitational settling or electrostatic mechanism. (The latter one occurs if a particle or a fiber or both elements carry some charges.) For neutral fibers and neutral nanosized and submicrometer particles (such conditions are considered in this paper) the primary mechanisms that affect the particles' deposition are diffusional and direct interception ones; however, inertial impaction mechanism can also influence the deposition efficiency of a bit larger particles. Utilizing the commonly used classical single fiber theory developed for the Kuwabara cell model [14], the single fiber filtration efficiency due to a separate action of these particular mechanisms can be estimated from the correlations proposed, e.g., by Stechkina and Fuchs [15] for the diffusional mechanism:

$$E_D = 2.9\left(\frac{1-\alpha}{Ku}\right)^{1/3} Pe^{-2/3} \tag{1}$$

and by Lee and Gieseke [16] for the interception mechanism:

$$E_R = \frac{(1-\alpha)}{Ku}\frac{N_R^2}{(1+N_R)^m}, \tag{2}$$

where $m = 2/[3(1-\alpha)]$. Note, that theoretically derived numerical constant 2.9 in Eq. (1) is sometimes replaced with a lower value (2.6 or 1.6) to obtain a better agreement of the theory with experiments, e.g., Lee and Liu [17,18]. This is due to the fact that the Kuwabara cell model does not take into account possible inhomogeneity of a filter internal structure related to a nonuniform distribution of the fibers in a space (variation in local porosity) or to a polydispersity of the fibers' sizes.

In the above formulae, α denotes the filter packing density, Ku is the Kuwabara hydrodynamic factor: $Ku = -0.5\ln\alpha - 0.75 + \alpha - 0.25\alpha^2$, N_R is the interception parameter: $N_R = R_P/R_F$, where R_P and R_F are radii of a particle and a fiber, respectively, and Pe means the Peclet number:

$$Pe = \frac{2R_F U_0}{D}. \tag{3}$$

U_0 denotes the air velocity, and D is a particle diffusion coefficient that can be expressed as:

$$D = \frac{k_B T}{f}. \tag{4}$$

Here k_B is the Boltzmann constant, T denotes absolute temperature, and f is the particle friction coefficient, which for a spherical particle is given by:

$$f = 6\pi\mu_g R_P/C_C. \tag{5}$$

In the above equation μ_g is the gas viscosity, and C_C denotes the Cunningham slip correction factor that is calculated as:

$$C_C = 1 + Kn_P\left[a_{Cc} + b_{Cc}\exp(-d_{Cc}/Kn_P)\right], \tag{6}$$

where the Knudsen number for a particle, Kn_P, is defined in the following way:

$$Kn_P = \frac{\lambda_g}{R_P}, \tag{7}$$

and λ_g is the gas mean free path. The values of the a_{Cc}, b_{Cc}, and d_{Cc} coefficients in Eq. (6) may be found in the literature. Allen and Raabe [19] quoted the following coefficients' values: $a_{Cc} = 1.142$, $b_{Cc} = 0.558$, $d_{Cc} = 0.999$.

Theoretical correlations for the single fiber efficiency due to the inertial impaction are less accurate. One of the frequently referred formula was proposed by Yeh and Liu [20]:

$$E_I = \frac{Stk\,J}{2Ku^2}, \tag{8}$$

where $J = (29.6 - 28\alpha^{0.62})N_R^2 - 27.5N_R^{2.8}$ and Stk is the Stokes number, which for a spherical particle is defined as:

$$Stk = \frac{R_P^2 U_0 \rho_P C_C}{9\mu_g R_F}. \tag{9}$$