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Pressure drop model for nanostructured deposits

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ABSTRACT

This study presents a new pressure drop model developed for cakes composed of nanostructured particles. The cake structure is understood as a tangle of chains composed by juxtaposed primary particles with (aggregates) or without (agglomerates) a partial overlap. Since cake porosity is one of the main parameters determining aeraulic resistance, an experiment protocol based on the changes in deposit thickness as a function of the cake mass per surface area has been developed to accurately determine this parameter. To this end, the pressure drop and the porosity of the cakes created by the filtration of carbon nanoparticles aggregates and agglomerates on PTFE membrane were measured. The aggregate and agglomerate count median mobility diameters range from 91 nm to 170 nm and from 48 nm to 62 nm, respectively. The associated Peclet numbers range from 0.19 to 53 for filtration velocities of 0.01, 0.05 and 0.09 m/s. Initial experimental results indicate that the porosity of the cakes ranges from 0.94 to 0.984 in correlation with the Peclet number of the aggregates or agglomerates. The agreement between experimental results and the pressure drop model is fairly good. Of the experimental values, 95% are within plus or minus 25% of the theoretical value.

1. Introduction

The manufacture of nanoparticles is increasing and opens up possibilities for new applications and economical developments. According to Roco et al. [1], the worldwide nanomaterials marketplace in 2020 will represent a $3 trillion market associated with nearly 6 million workers. Nevertheless, these economical concerns should not overshadow the social impact of nanoparticles, and research must be led on the toxicity of such products. Due to this social concern, the containment of airborne nanoparticles and hazardous particulate matter during production processes is essential in order to reduce worker exposure as much as possible and protect the environment. Fibrous media are a widely used solution, and the question of penetration of nanoparticles through the media [2–4] and clogging [5,6] of filters is still being investigated.

On the other hand, the Fukushima event reminded our society of the critical subject of nuclear installation containment. In most cases this containment is achieved using a ventilation system and High Efficiency Particulate Air (HEPA) filter to create sub-atmospheric pressure in the facility. In the case of fire, soot particles emitted could rapidly clog the HEPA filters on the ventilation ducts and, as a consequence, modify the ventilation conditions inside the installation. Among other things, the specific morphology of soot [7] creates challenges when describing the behaviour of HEPA filters in case of fire. Recent research conducted by IRSN [8,9] provides for the description of the complex clogging behaviour of HEPA filters in fire conditions according to an empirical model. Nevertheless, such approach is limited and most of the previous studies have focused on specific fire conditions or the filtration of micronic particles in ambient temperature and pressure conditions. To our knowledge, studies investigating the pressure drop of nanoparticle cakes are limited [10,5,11] and the phenomenological description of the clogging phenomena for nanoparticle aggregates has been poorly investigated.

Several correlations used to estimate the pressure drop of the cake can be found in the literature. They can be divided in two groups: the capillary model and the particulate model. The most popular correlation based on the capillary model is the Kozeny–Carman equation in Stokes regime. In this approach, the porous medium is considered to be an assembly of capillaries of specific size and geometry through which fluid flows. The particulate model is based on flow around particles. Mauret and Renaud [12] and more recently Puncochar and Drahos [13] have determined the applicability range of these models. In the case of fibre beds, Mauret and Renaud [12] show that the capillary approach is less suitable for porosities greater than 0.75 and for Reynolds numbers below 100. Since the porosity of nanostructured deposits is very

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List of variables

Cc	slip correction factor (–)
Co	overlap parameter (–)
$\overline{Co,p}$	mean 2D projected overlap coefficient (–)
D	aggregate or agglomerate diffusion coefficient ($m^2\ s^{-1}$)
d	distance between the centres of two particles in contact (m)
d_{agg}	aggregated or agglomerated particle size (m)
d_p	fibre or particle diameter (m)
d_{pG}	count median diameter (m)
d_{vg}	geometric mean size of the volume equivalent diameter (m)
Fc	correction factor (–)
F_T	drag force per unit length of fibre acting on fibres ($N\ m^{-1}$)
L	total length of fibres per deposit surface area (m^{-1})
M_c	deposited mass of nanoparticles (kg)
m_S	cake mass per surface area ($kg\ m^{-2}$)
N	number of primary particles per cubic meter of cake (–)
Pe	peclet number of aggregates/agglomerates (–)
Uf	gas velocity ($m\ s^{-1}$)
V_{pp}	volume of the primary particle (m^3)
Z	nanostructured deposit or filter thickness (m)
α	packing density of the nanostructured deposit ($\alpha = 1 - \varepsilon$) (–)
ΔP	pressure drop of a nanostructured deposit (Pa)
ε	porosity of the nanostructured deposit ($\varepsilon = 1 - \alpha$) (–)
ς_1, ς_2	empirical constants ($\varsigma_1 = 1.1 \pm 0.1$ and $\varsigma_2 = 0.2 \pm 0.02$ for $D_f \approx 1.78$, [19])
κ	dynamic shape factor of the particles (–)
λ	mean free path of gas (m)
η	gas viscosity (Pa s)
ρ_p	particle density ($kg\ m^{-3}$)
σ_g	geometric standard deviation of particle size distribution (–)
$v(\alpha)$	void function (–)
Ω	filtration surface area (m^2)

high, ranging from 90% to 98% [14,5,11], the approach based on capillary model is not relevant.

The particulate model developed by Endo et al. [15] is currently widely used to determine the pressure drop of a nanostructured deposit. In this approach, the pressure drop across a particle layer is assumed to be equal to the fluid drag acting on all individual particles. For a particle size distribution following a log normal distribution and in a Stokes regime, the authors obtained the following expression:

$$\Delta P = 18\frac{\eta Uf}{Cc}\frac{v(\alpha)}{(1-\alpha)^2}\frac{\kappa}{d_{vg}^2\exp\left(4ln^2\sigma_g\right)}\frac{m_s}{\rho_p} \qquad (1)$$

where η is the gas viscosity, α the packing density (α = 1 − Porosity (ε)), d_{vg} the geometric mean size of the volume equivalent diameter, σ_g the geometric standard deviation of particle size distribution, Cc the slip correction factor, Uf the gas velocity, ρ_p the particle density, $v(\alpha)$ the void function, κ the dynamic shape factor of the particles and m_S the cake mass per surface area. It should be noted that the void function makes it possible to take the effect of neighbouring particles into account.

Kim et al. [5] and more recently Liu et al. [11] have shown that the Endo's model is applicable for soot agglomerate deposits since it takes into account the size distribution of the spherical primary particles (κ = 1) and not the size distribution of the agglomerates. Note that the authors have used different void functions without justifying their choice. Moreover, Kim et al. [5] used the void function defined as $v(\alpha) = 10\ (1-\varepsilon)/\varepsilon$ although, according Endo, it is only applicable in the porosity range from 0.3 to 0.6. However, Endo's model does not take into account the partial overlapping of particles making up the cake although the SEM images provided by the authors seem to prove its existence.

The goal of this work is to investigate and evaluate the porosity of the cake layer formed by aggregates or agglomerates of nanoparticles and to develop a predictive pressure drop model taking into account the overlap between primary particles observed for aggregates.

2. New pressure drop model

Endo et al. [15] determined the pressure drop of a particle deposit from the sum of the drag forces acting on all the particles forming the cake. However, the nanostructured deposit can be understood as a tangle of chains composed by juxtaposed particles with (aggregates) or without (agglomerates) partial overlapping (Fig. 1). It therefore makes more sense to use the drag force acting on the chain of particles rather on particles. Sakano et al. [16] defined the drag force per unit length of fibre acting on fibres using the Davies equation [17]:

$$F_T = \frac{16\pi\alpha^{0.5}(1+56\alpha^3)}{Cc}\eta Uf \qquad (2)$$

where α is the packing density ($\alpha = 1 - \varepsilon$), η the air viscosity, Uf the air velocity and Cc the Cunningham coefficient defined as follows:

$$Cc = 1 + \frac{2\lambda}{d_p}\left[a + b\exp\left(-\frac{cd_p}{2\lambda}\right)\right] \qquad (3)$$

where a = 1.165, b = 0.483, c = 0.997 [18] and λ, the mean free path (in air at 20 °C and atmospheric pressure λ = 66.4 nm).

The pressure drop of a fibrous filter is equal to:

$$\Delta P = F_T L \qquad (4)$$

where L is the total length of fibres per deposit surface area.

To calculate L, we have to take into account the structure of the deposit. For a fibrous filter characterized by a fibre diameter (d_p), a thickness (Z) and a packing density (α), L is equal to:

$$L = L_F = \frac{4\alpha}{\pi d_p^2}Z \qquad (5)$$

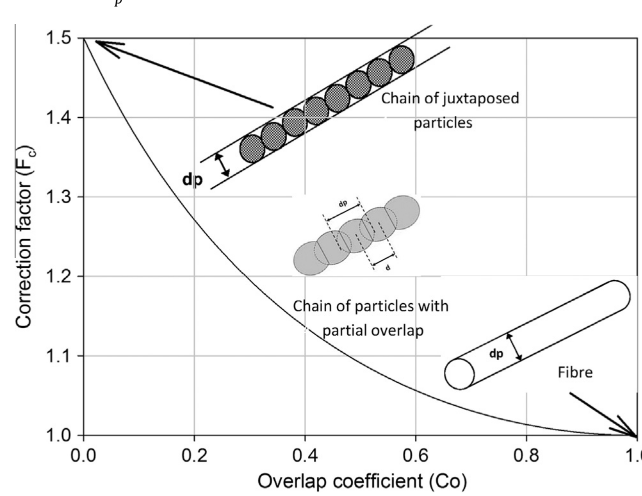

Fig. 1. Correction factor (Fc) versus overlap coefficient (Co).