Effect of Filter Inhomogeneity on Deep-Bed Filtration Process – A CFD Investigation

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ABSTRACT: Aerosol filtration in fibrous filters is one of the principal methods of removal of solid particles from the gas stream. The classical theory of depth filtration is based on the assumption of existing single fiber efficiency, which may be used to the recalculation of the overall efficiency of the entire filter. There are several reasons for inappropriate estimation of the single fiber efficiency including the assumption of the negligible effect of the presence of neighboring fibers and perpendicular orientation of the homogenous fibers. This work aims to investigate the influence of mesoscale inhomogeneity on fibrous filter performance using Computational Fluid Dynamics in models of filters differed by internal structure.

KEYWORDS: Brownian dynamics; Aerosol mechanics; Filtration.

INTRODUCTION

Aerosol particles are present in many industrial processes. One of the principal methods of their accurate removal from a gas stream is filtration. The classical theory of depth filtration of aerosol particles in fibrous structures is based on the assumption of existing single fiber efficiency, E, which may be used to a recalculation of efficiency of the entire filter. Using the classical theory of filtration may introduce some errors. There are several reasons for inappropriate estimation of the single fiber efficiency: i) neglecting the short-range interactions, ii) artificial separation of the inertial and Brownian effects, iii) assumption of perfect adhesion of particles to the fiber, iv) assumption of perfect mixing of aerosol particles in the gas stream, v) assumption of the negligible effect of the presence of neighboring fibers and vi) assumption of the perpendicular orientation of the homogenous fibers in the filter structure. The aim

of this work is to investigate the influence of mesoscale inhomogeneity on fibrous filters performance using Computational Fluid Dynamics calculations in models of filters differed by internal structure.

THEORETICAL SECTION

Filter inhomogeneity

The first approach to modeling the mesoscale inhomogeneity was purely empirical correction factors, derived to obtain agreement between theory and experiment[1]. These correction factors (called filter inhomogeneity factors) for pressure drop, ΔP , and efficiency, η , are defined as:

$$\Lambda_{\rm P} = \frac{\Delta \rm P}{\Delta \rm P_{hom}} \tag{1}$$

$$\Lambda_{E} = \frac{\ln(1-\eta)}{\ln(1-\eta)_{hom}} \tag{2}$$

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Cai [2] reported the following expressions:

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$$\Lambda_{\rm P} = \exp\left(-3\sigma_{\rm p}^2\right) \frac{0.4\sigma_{\rm p}^3}{0.8 + \sigma_{\rm p}^3} \tag{3}$$

$$\Lambda_{\rm E} = \exp\left(-2\sigma_{\rm p}^2\right) \frac{0.8\sigma_{\rm p}^3}{1.3 + \sigma_{\rm p}^3} \tag{4}$$

Where σ_p is relative standard deviation of pore size distribution.

Shweers and Löffler [3] subdivided a filter into a series of cubical elements with different local permeabilities and then used the known correlations for the single fiber deposition efficiency for each element. The distribution of local packing densities was assumed to be the log-normal. The overall filter efficiency was then calculated element by element. A similar approach was used by Dhaniyala and Liu [4]. The authors also, assumed the log-normal distribution of local packing densities and used well known correlations to calculate single fibre efficiency as a function of the local packing density. The filter efficiency was then obtained computing the integral-mean of the deposition efficiency averaged over the assumed distribution of the packing density. An even simpler model was proposed by Clement and Dunnett [5]. The authors used the standard equation of the classical theory of filtration,

$$1 - \eta = \exp(-\lambda L) \tag{5}$$

where L is filter depth, assuming that for a nonuniform filter the parameter λ is a random variable (along various paths through a filter) having Gaussian distribution.

All these models can predict a lower pressure drop and a higher penetration than results from the "classical theory" for homogeneous structures. Neither of them, however, seems to be realistic, since they are based on the concept of the single fiber efficiency and averaging over an assumed distribution. Thus, the effect of neighboring fibres is in practice neglected. Moreover, as the transport of aerosol in a porous space between many fibers is not considered

in these models, the fundamental phenomena related to the filter nonuniformity (namely, a preferential "channeling" of flow through regions of a higher local porosity and the "shadowing" of fibers by preceding ones in zones of a lower local porosity) are not taken into consideration. *Podgórski* and *Moskal* [6] and *Podgórski* [7] have performed 2D analysis for a representative volume of a filter, which contains a small enough number of fibers to enable a numerical solution of microscopic transport equations, and simultaneously large enough to assure that the results obtained are statistically significant. *Przekop* and *Podgórski* [8] have shown the strong mutual fibers orientation effect on deposition efficiency and spatial distribution of deposited particles.

Numerical simulations became the important source of information on filter performance over the last decade [9-15]. Recently *Ansari et al.* [16] have compared the deposition efficiency of aerosol particles in two configurations of fibers. The laminar flow in the filter was simulated using lattice-Boltzmann method. *Babaie Rabiee et al.* [17] have studied characteristics of two dimensional arrangements of fibers (parallel, staggered and random). Similar analyses were performed by *Banihashemi-Teherani et al.* [18].

The model

In order to analyze theoretically the effect of local mesoscale filter inhomogeneity on filter macroscopic characteristics nine various 3D model structures were generated, each one having the same mean porosity and consisting the same number of identical parallely oriented fibers placed in rectangular unit cells (Fig. 1). The size of the unit cell can be calculated from:

$$x_{cell} = y_{cell} = \sqrt{\frac{\pi}{\epsilon}} \frac{d_F}{2}$$
 (6)

Where ε is filter porosity and d_F fiber diameter. The length of the fibers was 50 μ m.

These structures had a different spatial distribution of the fibers. The structures were generated as slightly disturbed ordered structures. . They corresponded to the widely used models of a fibrous filter: channel model (rectangular array) with stochastic displacements generated as random variables having Gaussian distribution with zero mean and assumed standard deviations (Fig. 1). The studied structures were composed of 100 unit cells (20 in the main direction of gas flow by 5 in the perpendicular one) with diameter equal to 10 μm differed by mean porosity and standard deviation of fibres displacement. Stochastic displacements Δx and Δy

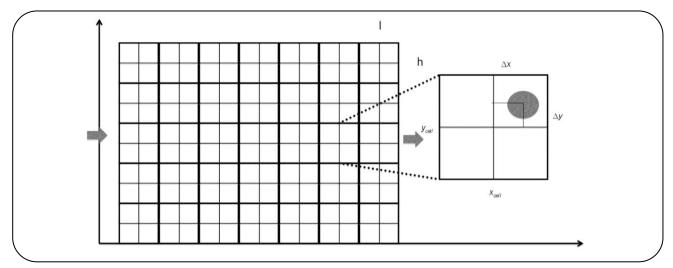


Fig. 1: Cross section of the filter structure.

were generated as random variables having Gaussian distribution with zero mean and assumed standard deviation, σ . The displacement of the fiber was calculated as a product of generated random number and size of unit cell. The geometrical parameters of filter structures are summarized in Table 1.

For the nine generated structures the gas flow patterns were determined numerically using the commercial CFD package Ansys Fluent finite volume analysis. Gas properties were taken as for air at p=101325 Pa and T=300 K. Calculations were performed for the inlet gas velocity equal to 0.02 m/s. The Reynolds number related to the considered velocity inlet was equal to 1.0, so laminar flow in the system could be assumed and no turbulence modeling was needed.

The computational domain was created in ANSYS ICEM 17 and the numerical meshes in all cases consisted of about 1 200 000 tetrahedral cells. The grid was the densest in the regions where the large gradients of velocity were predicted It was checked that the results of computations were not sensitive to a further increase of the number of cells.

To reduce complexity of the problem, the steady flow assumption has been made. Second-order upwind discretization was used for the convection terms in the momentum equations, while the SIMPLE method was used to solve the pressure–velocity coupling. The flow was initialized using the velocity values at the inlet plane. The boundary conditions at the exit from the object were of the "OUTFLOW" type; that is the velocity gradients

and pressure components, normal to the cross-sectional planes at the exit, were equal to zero. The air velocity at the walls was also zero. Symmetry boundary conditions were used on the top and bottom sides of the considered geometry due to possibility of reduce the extent of computational model and using better quality of calculation grid. The iteration process was terminated once the residual of the mass balance and all velocity components fell down below a predefined convergence criterion (10^{-6}).

Determination of structures of deposited particles on the filter fibre requires the knowledge of a history of the individual particle and its position and velocity vectors. The Lagrangian method of analysis should be used for description of the process. Particle trajectory is calculated for the generalised Besset-Boussinesqu-Ossen equation, which in simplified form is reduced to the expression:

$$m\frac{dv}{dt} = F^{(D)} + F^{(ext)} + F^{(R)}$$
 (7)

where $F^{(D)}$, $F^{(ext)}$ and $F^{(R)}$ are drag, external and random Brown forces, respectively.

Foundations of the Brownian Dynamics were established by *Chandrasekhar* [19] for a Stokesian particle in stationary fluid and for a force-free field. In this work extension of BD for the case of moving fluid at presence of the external forces derived by Podgórski [7] was used. Integration of the equation (7) for the time interval Δt , small enough that the host fluid velocity u_i and external force $F_i^{(ext)}$ may be assumed constant over

porosity, ε [-]	standard deviation of fibre displacement, $\sigma\left[\text{-}\right]$	filter depth, L [mm]	Filter height H [mm]
0.99	0.1	1.773	0.443
0.99	0.5	1.773	0.443
0.99	2.0	1.773	0.443
0.95	0.1	0.991	0.248
0.95	0.5	0.991	0.248
0.95	2.0	0.991	0.248
0.90	0.1	0.561	0.140
0.90	0.5	0.561	0.140
0.90	2.0	0.561	0.140

Table 1: Parameters of investigated filters.

 $(t,t + \Delta t)$, gives the following bivariate normal density probability distribution functions $\varphi_i(\Delta v_i, \Delta L_i)$ that during time interval Δt the particle will change its i^{th} component of velocity by Δv_i and it will be displaced by the distance ΔL_i in i^{th} direction.

$$\begin{split} & \phi_{i} = \frac{1}{2\pi\sigma_{v_{i}}\sigma_{Li}\sqrt{1-\rho_{c}^{2}}} exp \left\{ \frac{1}{2\left(1-\rho_{c}\right)^{2}} \left[\left(\frac{\Delta v_{i} - \left\langle \Delta v_{i} \right\rangle}{\sigma_{Li}} \right) - \left(8 \right) \right. \\ & \left. - \frac{2\rho_{c} \left(\Delta v_{i} - \left\langle \Delta v_{i} \right\rangle \right) \left(\Delta L_{i} - \left\langle \Delta L_{i} \right\rangle \right)}{\sigma_{v_{i}}\sigma_{Li}} + \left(\frac{\Delta L_{i} - \left\langle \Delta L_{i} \right\rangle}{\sigma_{Li}} \right)^{2} \right\} \right] \end{split}$$

The generalised algorithm for the Brownian dynamics can be formulated as follows. For a given initial particle position and its initial velocity components, v_i , at a moment t, one calculates the local fluid velocity, u_i , the external forces, $F_i^{(ext)}$, then, one determines the expected values $\langle \Delta v_i \rangle$ and $\langle \Delta L_i \rangle$ and the correlation coefficient, ρ_c . Next, we generate two independent random values G_{Li} , G_{vi} , having Gaussian distribution with zero mean and unit variance. Finally we calculate the change of particle velocity, Δv_i , and the particle linear displacement, ΔL_i , during time step Δt from the expressions accounting for deterministic and stochastic motion:

$$\Delta v_{i} = \langle \Delta v_{i} \rangle + G_{vi} \sigma_{vi} \tag{9}$$

$$\Delta L_{i} = \left\langle \Delta L_{i} \right\rangle + \rho_{c} G_{vi} \sigma_{Li} + \left(1 - \rho_{c}^{2}\right) G_{Li} \sigma_{Li} \tag{10}$$

All the steps are repeated for each co-ordinate i = 1, 2, 3. Having determined the increments Δv_i and ΔL_i the new particle velocity at the moment $t + \Delta t$ is obtained as

 $v_i(t+\Delta t) = v_i + \Delta v_i$, and in the same manner the new particle position is calculated. After completing one timestep of simulations, the next step is performed in the same way.

RESULTS AND DISSCUSSION

The aim of this study was to compare the initial filtration efficiency of filters with different level of inhomogeneity with one calculated using classical filtration theory independence rule. We have decided to keep the number of fibers in computational domain constant, instead of e.g. the filter thickness, as the main purpose was to find the general relation between the level of inhomogeneity and filtration efficiency, not the prediction of real filter performance. Moreover, the total surface of collectors open for deposition was kept constant for all the cases. The single fiber efficiency, *E*, was thus calculated from

$$E = 1 - (1 - E_D)(1 - E_I)(1 - E_R)$$
(11)

where E_D , E_R and E_I are single fiber efficiency due to diffusive, inertial and direct interception mechanisms, respectively. The formula for E_D was given by *Stechkina* and *Fuchs* [20]

$$E_{\rm D} = 2.9 \text{Ku}^{-1/3} \text{Pe}^{-2/3} \tag{12}$$

where Ku is Kuwabara factor and Pe, Peclet number. Kuwabara factor is a function of filter packing density, α

$$Ku = -\frac{\ln \alpha}{2} - \frac{3}{4} + \alpha - \frac{\alpha^2}{4} \tag{13}$$

$$Pe = \frac{ud_f}{D} \tag{14}$$

Where u is superficial gas velocity and D is diffusion coefficient of particle.

Inertial impaction occurs when the particle, because of its inertia, is unable to adjust quickly to the abruptly changing streamlines near the fibre and crosses those streamlines to hit the fibre. The parameter that governs this mechanism is Stokes number

$$Stk = \frac{\rho_p dC_C U}{18\mu d_F}$$
 (15)

The single fibre efficiency for inertia was given by *Yeh* and *Liu* [21]

$$E_{I} = \frac{StkJ}{Kv^{2}}$$
 (16)

where:

$$J = (29.6 - 28\alpha^{0.62})R^2 - 27.5R^{2.8}$$
 (17)

for
$$R < 0.4$$
 $J = 2.0$ for $R > 0.4$

Impaction is the most important mechanism for large particles. But such particles reveal significant collection by direct interception as well. The sum of E_I and E_R may not exceed theoretical value of R+1.

The single fibre deposition efficiency due to interception depends on the dimensionless parameter, R, defined as

$$R = \frac{d_p}{d_F} \tag{18}$$

The single fibre efficiency due to interception was given by *Lee* and *Ramamurthi* [22] as:

$$E_{R} = \frac{\left(1 - \alpha\right)R^{2}}{Ku\left(1 + R\right)} \tag{19}$$

The results of filtration effciency for filters with different porosity are presented in Fig. 2. The overal filter efficiencies were calculated form Eq. (5). Parameter λ may be obtained from

$$\lambda = \frac{4E}{\pi d_{\rm F}} \left(\frac{1 - \varepsilon}{\varepsilon} \right) \tag{20}$$

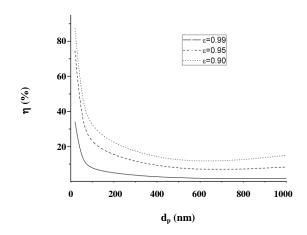


Fig. 2: Filtration efficiency for different porosities.

The effect of inhomogeneity level on filtration efficiency for filters with different porosity is presented in Figs. 3-5. The results are ensemble average from 10 series of calculations of 1000 particles trajectories for each case. The filtration efficiency was calculated as a ratio of number of particles deposited on fibers to the number of particles admitted to the computational domain. The perfect adhesion was assumed, what means that the particle that touches the surface of the collector is deposited and there's no possibility of reentrainment. For small (submicron) particles Brownian diffusion is predominant mechanism of deposition, while for big ones (with diameter larger than 1 µm) interception and inertia plays the major role. One can observe the minimum value of filtration efficiency for particles of diameter around 500 nm, where none of the deposition mechanisms is efficient. For the filter with 0.99 porosity the highest values of filtration efficiency for the whole range of particles diameters are observed for the filter with most inhomogeneous structure. The biggest effect of filter inhomogeneity is observed for most penetrating particles. For the filter with 0.95 porosity, one can also observe the highest value of filtration efficiency for most inhomogeneous filter, but the effect is not that significant as for previous case. Finally, for the filter with 0.9 porosity the highest value of filtration efficiency is observed for intermediate level of filter inhomogeneity. Fig. 6 shows the relation between the inhomogeneity factor and particles diameter for filters with different highest level of inhomogeneity. One can observe that for small particles Λ_E is smaller

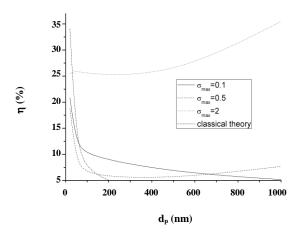


Fig. 3: The effect of inhomogeneity level on filtration efficiency, ε =0.99.

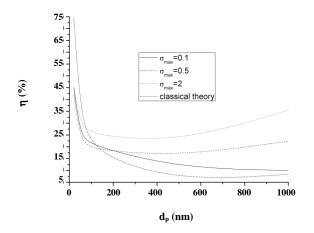


Fig. 4: The effect of inhomogeneity level on filtration efficiency, ε =0.95.

than 1 and increases with particle diameter. The highest influence of filter inhomogeneity on filtration efficiency is observed for the filter with highest porosity.

CONCLUSIONS

Transport and deposition of aerosol particles in random fibrous filter structures were analysed. The results of numerical simulations show that the "classical theory" of depth filtration based on the concept of constant single fibre efficiency is inappropriate and causes significant error in the estimation of the filter efficiency.

Numerical simulations indicate the significance of local structural inhomogeneities of fibrous filters. As a result, flow passes through preferential pathways of higher local porosity and the "screening" effect of fibers

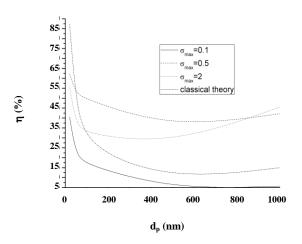


Fig. 5: The effect of inhomogeneity level on filtration efficiency, ε =0.9.

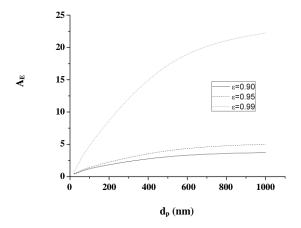


Fig. 6: Effect of particle diameter on inhomogeneity factor.

by preceding ones occurs in the regions of higher local packing density. Consequently, local deposition rates of aerosol particles are unevenly distributed in the filter. Limited level of inhomogeneity may increase filtration efficiency.

The inhomogeneity factor for penetration was found to be dependent on particle diameter; thus, existing correlations, which account only for filter structural characteristics, seem not to be generally valid.

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