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Introduction to Basics of Submicron Aerosol Particles Filtration Theory via Ultrafine Fiber Media

N.A. Hakobyan
A.I.Alikhanian Yerevan Physics Institute, Yerevan, Armenia

E-mail: h.narek@yerphi.am

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Abstract - The deposition of aerosol particles in ultrafine fiber media under the action of different mechanisms (sieving, interception, diffusion, inertia, gravitational and van der Waals forces, etc.) is considered taking into account their own sizes. The modeling of fine filtration process has shown high sensitivity of the capture coefficient to the changes in flow rate, viscosity, particle and fiber parameters, as well as to packing density of the fiber system are the reasons for the relative growth of efficiency of high-performance filters based on ultrafine fiber media.

Keywords: Filtration, ultrafine, fiber, aerosol, deposition, efficiency.

1 . Introduction

The need to study the process of fine filtration of submicron aerosols by ultrafine fibers of 0.1-2*mkm* in diameter is due to stringent requirements to gas and radionuclide purity when solving a wide complex of urgent problems, such as development of new technologies for reducing hazardous emissions into the environment. Modern fine fiber filters reveal the least flow resistance at a certain particle capture efficiency as compared with other filter materials (carbon filters, Petryanov filters), and therefore they can receive wide acceptance for gases and supply air cleaning in high-radiation areas and admissible control zones, for example, those on the basis of ultrafine modified basalt fibers that meet the specified requirements of cleaning (in respect of efficacy and resistance) [1].

The existing theoretical understanding of the mechanisms of particle deposition and accumulation of particles in filters and filtration models are mostly empirical and do not allow assessing, within the required accuracy, the effectiveness of particle capture or predicting the filter resources without additional experimentation. Further development of theoretical ideas is about physical mechanisms of particle capture. New mathematical models and methods are needed for reasonably choosing the parameters of high-performance filters, predicting the filter resources, choose the test conditions and improving filters.

The theoretical calculation of filter efficiency is a complex multi-factorial task and requires simultaneous consideration of own sizes of submicron particles and fibers, especially in the case of constrained and varied flow fields in the course of particles deposition on fibers. Despite more than a half-century history of the theory of aerosol filtration, the tasks related to quantitative estimation of various mechanisms of deposition of submicron particles and their accumulation in the filter media, are still not completely cleared. This is due, first, to the uncertainty of the flow field near the surface because of disordered internal structure of real filters, and second, necessity for considering many parameters of particles, fibers and the surrounding environment when calculating their deposition from the flow. Therefore, the particle deposition should be preferably studied on model filters that can adequately represent the basic properties of real filters [2].

2. Fundamentals and Mechanisms of Aerosol Filtration

To achieve "fine cleaning" it is necessary to have a material that provides the desired efficiency of particle capture at minimum flow resistance. The filter resistance is the pressure drop across the filter, Δp, divided by flow velocity before filter, U, and air dynamic viscosity, μ:

$$LF = \frac{\Delta p}{U\mu},$$

where L is the length of fibers per unit area of filter material: $L = \alpha H/\pi a^2$; α is the filter packing density (solid fraction), H is filter thickness, a is radius of the fiber; F is the dimensionless resisting force acting on a unit length of fibers.

The process of particle deposition on fibers is characterized by capture coefficient η. It is dimensionless deposition rate of particles per unit length of fibers in filter and is related to the filter efficiency E and penetration P by the following formulas:

$$P = {}^{N}/_{N_0},$$

$$E = 1 - {}^{N}/_{N_0} = 1 - \exp(-2a \cdot L\eta),$$

where N_0 and N are the particle concentrations before and after filter, correspondingly. To compare the initial characteristics of the filter is used the ratio of the logarithm of breakthrough to the pressure drop called "filter quality criterion":

$$\gamma = -\ln {}^{P}/_{\Delta p}$$

Paper [3] is devoted to the modeling of physical processes of filtration and the calculation of the of particles capture coefficient η by fiber. η is a function of many parameters: radius r_p and density ρ_p of captured particles; filter face velocity U; air temperature $T$and pressure p, the mean free path length of molecular gas particlesλ, availability of external forces F_e, filter parameters (thickness, packing density, average fiber radius a and its variance σ, as well as ε and w, parameters that characterize the internal structure of the filter and fiber shape respectively):

$$\eta = \eta\left(r_p, \rho_p, U, \mu, T, p, \lambda, F_e, a, \alpha, \sigma, \varepsilon, w, \ldots\right).$$

Furthermore, the capture coefficient is dependent on the electric charge q, the dielectric constant of the particles, availability of charges on fibers and dielectric constant of fiber material. For non-stationary filtration processes, after deposition of sediments on the fibers the capture coefficient will also depend on the amount of deposited particles and porosity β of the sediment [1,4-6].

Taking into account different mechanisms of particle deposition, the problem of determining the filter efficiency is reduced to the calculation of the capture coefficient depending on the filter parameters and several dimensionless parameters characterizing the filtering conditions:

$$\eta = \eta\,(Re, Kn, Kn_p, Pe, R, St, G, \ldots),$$

where $\mathrm{Re} = 2aU/\nu$ is Reynolds number; ν is kinematic viscosity of gas flow; $Kn = \lambda/a$, $Kn_p = \lambda/r_p$ are Knudsen numbers for fiber and particle respectively; $Pe = 2aU/D$ is the diffusion Peclet parameter, D is coefficient of particle diffusion; $R = r_p/a$ is the interception parameter; St is Stokes inertial parameter (see Inertial Mechanism); $G = U_G/U$ is the sedimentation parameter, U_G is the particle deposition rate.

First theoretical works were carried out on the basis of the flow field around an isolated cylinder [7]. However, for that time no quantitative agreement with experimental data calculations for the filters was obtained even for individual deposition mechanisms.

The history of filtration theory showed that the most acceptable model for flow in fibrous media is the "cell" model and was accepted by many authors in their fundamental works. Subsequently, many authors have investigated the cell model with different boundary conditions and were getting some different results [8-10]. A successful model proved to be a cell with Kuwabara boundary conditions [10] which was perfectly consistent with the experimental data [11-16].

The study of particle deposition was carried out using a model with a known flow field. As a model filter system, hexagonal pack of parallel fibers located perpendicularly to Stokes flow (*Re<<1*) direction was accepted. For high Reynolds numbers, the flow and Kuwabara cell models require additional theoretical conditions and reformulation [17]. In Kuwabara cell model the fibers are packed in a hexagonal arrangement (Fig. 1). Two of the boundary conditions are the radical and tangential velocities vanish at the fiber surface. The third condition is given by the fixed velocity at the $r = b$ and $\theta = \pi/2$ (Fig. 2). The fourth boundary condition used by Kuwabara was zero vorticity on the cylinder surface. Kuwabara assumed the positive vorticity on the upper side of the cell canceled with the negative vorticity on the bottom side of the cell, as shown in Fig. 1. Due to the simple form of the formulas for the forces of fiber resistance, stream function, velocity components and matching the experimental results, Kuwabara cell is widely used in solving many problems in the theory of filtration.

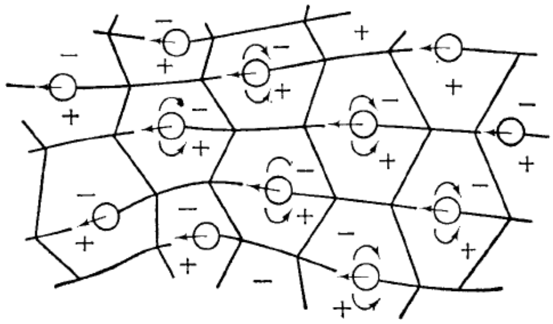

Fig. 1: In Kuwabara flow cell, fibers are packed in a hexagonal arrangement and vorticity is assumed to be zero on the cell bounding lines [19].

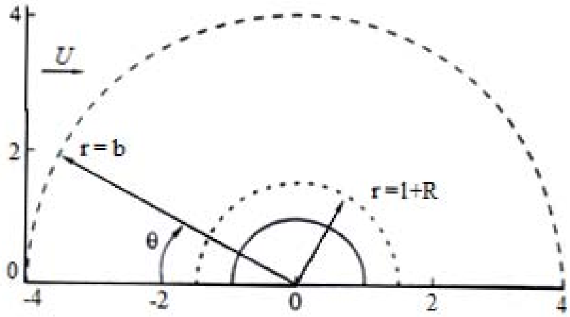

Fig. 2: Schematic layout of fiber in the cell, where $r = 1$ is dimensionless and matches fiber radius.

Unlike the Lamb solution for isolated cylinder [18], Stokes approximation for stream function in the case of parallel cylinders system does not depend on the Reynolds number, and is determined by the ratio of fiber diameter to the distance between cylinders or by the value of the cylinders system packing density as well.

A simplified method of finding solution of Navier-Stokes flow equations for low Re numbers (*Re<1*) is finding stream function ψ in this region. It can be obtained directly by solving the biharmonic equation in cylindrical polar coordinates:

$$\nabla^4\psi = 0, \qquad \psi = \left(Ar + \frac{B}{r} + Cr\ln r + Dr^3\right)\sin\theta$$

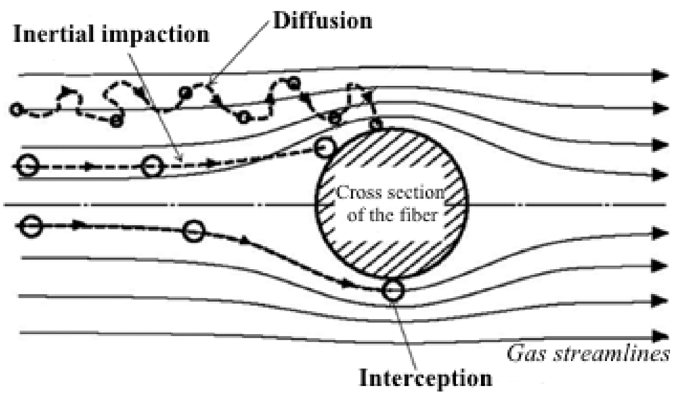

Fig. 3: Diffusion, inertial impaction and interception mechanisms of particle deposition on a fiber.

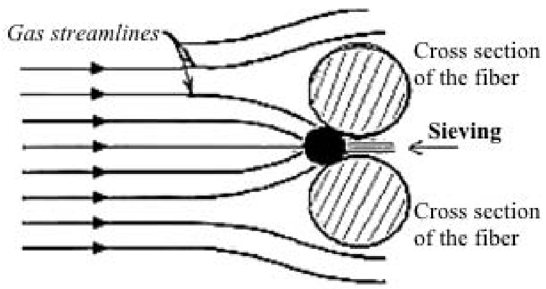

Fig. 4: Sieving mechanism of particle capture.

Here ψ is the simplest solution, and *A*, *B*, *C*, *D* can be obtained from the boundary conditions [19-20].

At least six different mechanisms of aerosol capture by fiber particles are known: sieving, engagement (interception), diffusion, inertial, also electric and gravitational (Fig. 3, 4). For capture by inertia impaction, interception, and electrostatic forces the single fiber efficiency (in cell) can be calculated from the equation of particle motion considering convective flow. Efficiency due to the convective Brownian motion can be calculated from the equation of convective diffusion with appropriate boundary conditions.

I. Sieving Mechanism

All particles having the radiuses more than half the distance between the fibers are completely retained by their frontal layer (Fig. 4). But this mechanism becomes valid and notable only when density of fibers is high. Also such filters become useless after a short time of the gas flow regime.

$$E_S = 1\ for\ r_p > d_{pore};\ E_S = 0\ for\ r_p < d_{pore}$$

where E_S is the efficiency of the sieve effect and d_{pore} is the pore diameter. The relation between fiber and pore diameter has according to Neckar [21] the following form:

$$d_{pore} = d_f \frac{\varepsilon}{1+w}\left(\frac{1-\alpha}{\alpha}\right)^{1/2}$$

where *w* is the fiber shape factor (zero for cylindrical fibers), ε is a constat related to the filter structure. For cylindrical fibers with hexagonal structure $\varepsilon = 2^{-1/2}$.

II. Interception (Engagement) Mechanism.

The second mechanism, interception or engagement, results in the capture of all particles moving along the flow lines, with the radius more than the distance of these lines from the fiber surface (see in Fig. 3). For isolated cylinders, the capture coefficient obtained from Lamb solution of Navier-Stokes flow equations for low *Re* numbers (*Re<1*) is [18]:

$$\eta_R = \frac{1}{2(2-lnRe)}[\,2(1+R)ln(1+R)-(1+R)+\,1/(1+R)].$$

According to the cell model [18, 22], the corresponding capture coefficient of particles for parallel cylinders depends on the radius and packing density of fibers, but does not depend on *Re*:

$$\eta_R = \frac{1+R}{2Ku}\left\{2ln\,(1+R)-1+\alpha+\left(1-\frac{\alpha}{2}\right)\,(1+R)^2-\frac{\alpha}{2}(1+R)^2\right\},$$

where $Ku = -{}^{3}/_{4} - {}^{1}/_{2}\,ln\alpha + \alpha - {}^{1}/_{4}\,\alpha^2$ is Kuwabara hydrodynamic factor. In most cases for fiber filter packages $\alpha \ll 1$ condition is true, therefore:

$$\eta_R = \frac{1}{2Ku}\left\{2(1+R)\,ln(1+R)-(1+R)+\frac{1}{(1+R)}\right\}, \tag{1}$$

It follows from (1) that a finer fiber is more efficient than a coarser fiber in intercepting the particles.

III. Inertial Impaction Mechanism.

The fourth mechanism is inertia caused by the displacement of aerosol particles with a finite mass from the flow lines curved near the fiber under the action of inertial force (see in Fig. 3). In this case the expression for the corresponding capture coefficient has the following form [3]:

$$\eta_I = \frac{St\cdot f}{2\,Ku^2}, \tag{2}$$

where $f = (29.6-28\alpha^{0.62})R^2-27.5R^{2.8}$ for *R<0.4* and *f = 2,* for *R>0.4* are empirical results [23-24]. A simple formula for *f* does not exist. The formula is valid for *0.004 <α< 0.1*.

The impact of inertia on deposition is determined by the Stokes number:

$$St = \frac{{r_p}^2\rho_p C_c U}{9\mu a},$$

where μ is dynamic viscosity of the flow and C_c is Cunningham slip factor correction for slip effect vanishing between gas and particle. This is important for the nano-sized particles when their diameters are comparable to the average length of the molecular path λ and it does not take into account the effect of the slip at the gas−fiber interface:

$$C_c = 1+\frac{1}{Kn_p}(1.257+0.4e^{(-1.1Kn_p)}),\;\; \lambda = \overline{R}T/4\sqrt{2}N_A{r_p}^2p,$$

where $\overline{R}, N_A, T, p$ are universal gas constant, Avogadro number, absolute temperature, gas pressure respectively. The mean free path is about 0.0645μm for air molecules.

If $St \gg 1$, particles continue moving and possibly will face fiber, and if $St \ll 1$, particles will move along the current line and the inertial effect will not take place.

Knudsen number for particles $Kn_p = {}^{\lambda}/_{r_p}$ is gas characteristic which determines its rarefaction by comparing the average mean path of molecules with characteristic dimensions of the environment, in this case, the particle radius. Four different modes can be distinguished in the gas stream, based on the value of Knudsen number: 1) free molecular mode, $Kn > 10$; 2) transitional mode: $0.25 < Kn < 10$; 3) slip mode: $0.001 < Kn < 0.25$; 4) continuous flow mode: $Kn < 0.001$.

For High Reynolds numbers the inertial effect becomes more appreciable and the streamlines approaching a fiber turn around more sharply [17].

IV. Diffusion Mechanism

The third mechanism is caused by Brownian diffusion of aerosol particles and their random collisions with the fiber surface out of flow lines at their path (see in Fig. 3).

For the system of ultra-thin fibers with a radius comparable with the average free path of gas molecules, the field of velocities and resistant force of fibers depend on Knudsen number.

The expression for the corresponding capture coefficient is obtained analytically in [25] and has the following form:

$$\eta_D = 2.9\, k^{-\frac{1}{3}}\, Pe^{-\frac{2}{3}}\left(1 + 0.39\, k\, Pe^{\frac{1}{3}}\, Kn\right), \quad (3)$$
$$k = Ku + 1.15\, Kn,$$

where $Kn = \lambda/_a$ Knudsen number for fiber; Pe is Peclet number of aerosol particle transportation, D is coefficient of Brownian diffusion and can be evaluated from the Stokes−Einstein expression at a given temperature T: $D = k_B TB$, where k_B is Boltzmann's constant; $B = \frac{C_c}{6\pi\mu r_p}$ is the mechanical mobility of a particle and is the inverse of the friction coefficient for a spherical particle.

V. Gravitational Deposition or Sedimentation (Settling) Mechanism

If the particle density is different from that of the fluid (it is assumed to be greater), then particles may settle out in the direction of the gravitational force. Capture coefficient for single fiber can be given by the following formula:

$$\eta_G = \frac{U_G}{U} = \frac{2{r_p}^2 g(\rho_p - \rho_{gas})}{9\mu U}, \quad (4)$$

where ρ_{gas} is gas density, g is free fall acceleration [26]. More detailed reference to th effect of gravity on particle motion and capture coefficient can be found in [27].

It can be seen from Fig. 5 that there are four main factors determining capture coefficients for single fiber, additive summing of which (see eq. 1-4) gives the qualitative shape of the overall efficiency curve and specifies its minimum value (the most penetrating particle). They are interception, inertial impaction, diffusion and gravitational settling.

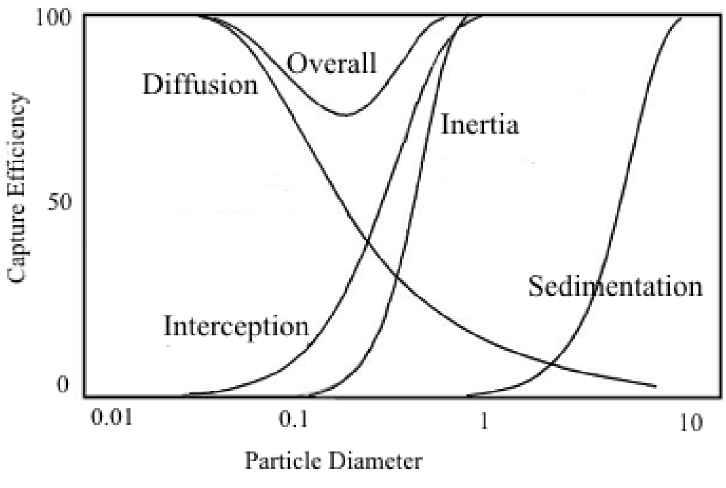

Fig. 5: The main four factors resulting total filter efficiency curve (qualitative demonstration).

VI. Electrostatic Forces

The fifth mechanism is caused by electrical forces between fibers and aerosol particles in the cases when they are charged. There are three possible cases of interaction: charge-charge, when particle and fiber are charged heteropolarly or unipolarly and attracted or repelled by Coulomb force, charge-dipole when either particle or fiber is charged and the charged object induces dipole in uncharged object by its electric field, and finally, dipole-dipole, when uncharged particle and fiber are located in an external electric field that induces in both objects dipoles attracting each other. As aerosol particles are often either uncharged or charged relatively weakly and strongly charged aerosol particles occur generally rarely, it is assumed that electric attraction plays a minor role in capture of aerosol particles. More detailed information about these mechanisms is given in [5].

VII. Impact of Van der Waals Forces

The deposition of aerosol particles takes place from a thin gas layer adjoining the ultrafine fiber. Therefore to model the particle capture process, an exact knowledge of aerosol flow and Van der Waals forces immediately near the ultrafine fiber surface is necessary.

It is known from the theory that two mechanisms of deposition, namely, Brownian diffusion and interception of particles are usually considered. However, an appreciable influence on the deposition of submicron particles on fibers exerts molecular Van der Waals forces. It is accepted to distinguish short-range Van der Waals forces, which operate at distances less than 0.01 *mkm*, and long-range forces (so-called "late forces") operating at approximately 0.1 *mkm* distances. Preliminary analysis has shown that the capture of particles from the stream is greatly determined by the late forces [28].

The formula for the capture coefficient upon the particle deposition caused only by Van der Waals forces derived in [28], has following form:

$$\eta_W = 0.573\left(\frac{A_7\, C_c\, r_p{}^2}{a^5\; U\; \mu\; Ku^{5/2}}\right)^{2/7}, \tag{5}$$

where A_7 is the constants of van der Waals interaction. The overall capture coefficient is determined by numerical integration of the equation of stationary convective diffusion (and it is not always an additive quantity). Fig. 6 shows the impact of Van der Waals forces on the capture coefficient as a function of particle radius, where η_{DRW} is an integral non-additive coefficient considering diffusion, interception and van der Waals forces and η_{DR} is without consideration of van der Waals forces. This impact is especially important near minimums of these curves, i.e. for the most penetrating particles. The consideration of Van der Waals forces leads to an appreciable increase in the capture coefficient, and in case of high A_7 values, to the displacement of the minimums towards smaller $r_p{}^*$ (the most penetrating particle) [29].

As it is seen from Fig. 7, the capture coefficient η_{DRGW} tends to zero with increase of fiber radius. At an essential influence of gravitation, the capture coefficient (without taking into account Van der Waals interactions) is negative, which is devoid of physical sense; hence, in this case it is lawlessly to consider the influence of sedimentation on the particle deposition without taking into consideration Van der Waals forces. It is evident that all other deposition mechanisms, how small their influence might be, would in this case be more notable. At the filtration of the aerosol flow directed from the top downward, Van der Waals interaction strengthens the sedimentation deposition and manifests itself in the lesser degree the stronger the gravitation is.

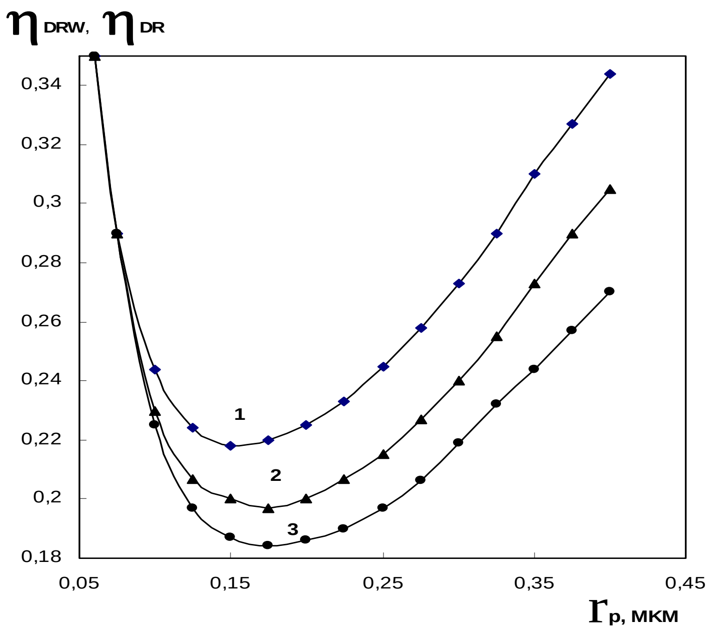

Fig. 6: Dependence of capture coefficient η_{DRW}(1,2) and η_{DR}(3) on particle radius at various interaction constants $A_7 = 10^{-18}$ erg.cm (1), $A_7 = 10^{-19}$ erg.cm (2), *a = 1 mkm, U =1 cm.s*$^{-1}$, α *= 1/16.*

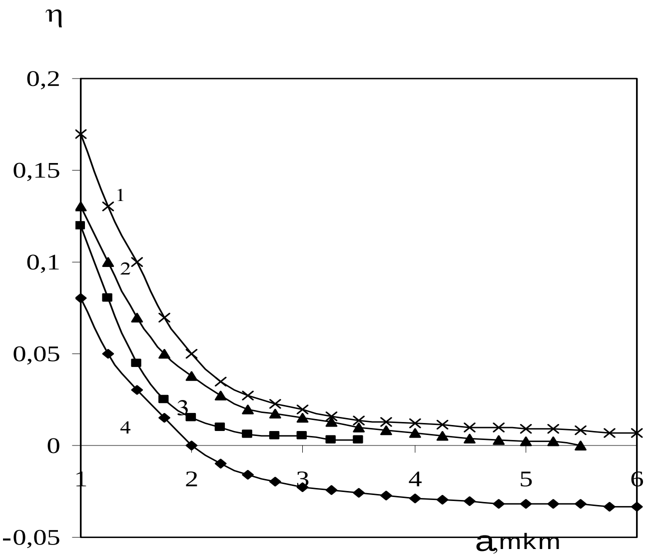

Fig. 7: Dependence of capture coefficients of particles with radius $r_p = 0{,}5$ mkm and density $\rho_p = 1 g/cm^3$ (1,2) and $10 g/cm^3$ (3,4) on fiber radius. Curves 2, 4 are calculated without taking into account Van der Waals interactions. $\alpha = 0{,}01$, *U =1 cm/s.*

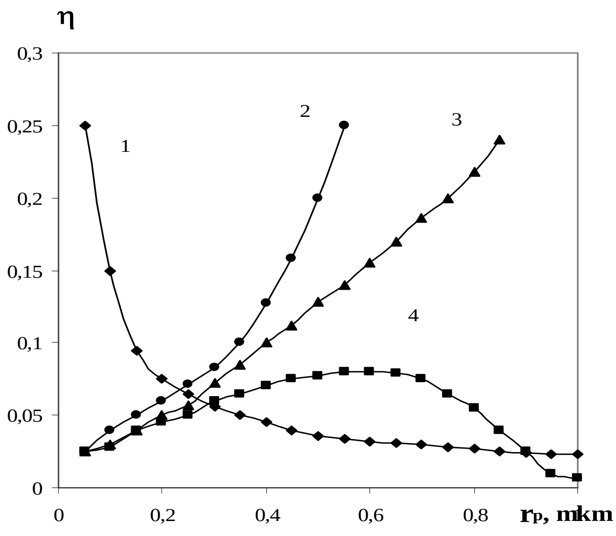

Fig. 8: Dependence of capture coefficient on radius of particles with density $\rho_p = 1 g/cm^3$ (2), $10 g/cm^3$ (3) and $20 g/cm^3$ (4). Curve 1 corresponds to diffusion capture coefficient. $\alpha = 0{,}01$, *a = 1 mkm, U =1 cm/s*

In such a filtration regime of high density (e.g. $\rho_p = 20g/cm^3$) particles in fiber media, when the influence of inertia (small Stokes numbers), diffusion and electric effects are small, the gravitational force can essentially influence the radius of the most penetrating particles. Unlike the non-gravitational case (Fig. 6), most penetrating particles with high density may have minimum at coarser particle radiuses, which is necessary to take into account when testing filters for aerosols with heavy particles at low flow velocities. Fig. 8 presents the examples of the calculation of overall η_{DRGW} depending on the radius, with maximum penetration radius over *1 mkm* (curve 4) [27].

3. Other Mechanisms

While the main mechanisms are dominant for submicron particles filtration, there are a few other mechanisms that might be important under some circumstances. These other mechanisms include the Saffman lift force, the thermophoretic force, the pressure gradient and particle-to-particle interaction, etc.

1. When solid particles just begin to deposit on a clean fiber, the captured particles scatter over the fiber surface sparsely. Smaller in size than a fiber and protruding further into the aerosol stream, a deposited particle is more efficient than a fiber in capturing particles. A dendrite or irregular chain-like aggregate is formed when a deposited particle captures another particle. Further deposition leads to growth of dendrites, which eventually bridge together to form a dust cake. For many types of filters, penetration decreases exponentially, whereas pressure drop increases exponentially with specific deposit (mass of particles captured per unit area of filter). Growth of dendrites and effects of particle loading on filter performance have been extensively studied for decades, but are not yet well understood [6,30].
2. A small particle in shear flow field experiences a lift force perpendicular to the flow direction due to the velocity gradient and inertial effects in the viscous flow around the particle. This force was reported by Saffman and thus called Saffman lift force [31]. For a viscous channel flow, the flow in the axial direction generates a Saffman lift force in the radial direction, which lifts the particles towards the center of the channel and gives relative importance to dominant forces. But it is usually considered to be important when a particle is fairly close to the surface, and is neglected for most studies.
3. Also, when a small particle is suspended in a gas that has a temperature gradient, the particle experiences a force in the direction opposite to the direction of temperature gradient. This phenomenon is called thermophoresis. This force is dependent on both the gas and particle properties, as well as the temperature distribution [32].
4. A particle striking a solid surface will rebound if the kinetic energy of the particle exceeds the adhesion energy and there is no energy loss during the impact. The threshold impact velocity above which rebound takes place is called the critical velocity [33].
5. For three relative humidity levels (0.04%, 1.22%, >92%) and face velocity of 0.025 ms^{-1}, the results showed that the filtration efficiency differed only slightly at different humidity levels. This is in contrast to larger particles, for which the collection efficiency increases with increasing humidity [34].

4. Conclusion

Based on the theoretical study of the modeling of aerosol particles deposition on ultrafine fibers, it is found that taking into account the basic mechanisms of capture of particles in combination with a certain amount of experimental data can help to predict the changes in the efficiency of filters depending on the existing prevailing operating conditions and requirements, for example in high-radiation areas of nuclear power plants.

Due to randomly arranged fibers in real filters, adjacent fibers have impact on the nature of their flow-past; fibers can touch each other and have the most diverse orientation, therefore it is impossible to apply a strictly mathematical equation for an isolated fiber. But in opposite, here was shown that there are several causes changing particle motion pattern around flow direction and causing deposition on fiber's surface with typical efficiency coefficients. Therefore, they can be calculated from integration of corresponding flow equations using different idealized models with specific boundary conditions.

It also should be noted that formulas presented in this work are mostly qualitative ones obtained analytically with empiric coefficients and grades. In general, the capture coefficients for a single fiber are not additive quantities. When summing, the same deposition event can be considered several times due to one or other effects because of interferences between those effects. That is why the exact quantitative estimations must be done by numerical calculation using extra information from literature.

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