

BROWNIAN DYNAMICS FOR CALCULATION OF THE SINGLE FIBER DEPOSITION EFFICIENCY OF SUBMICRON PARTICLES.

*In memory of Albert Podgórski who has initiated this work
and who passed away in December 2010*

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The motion of submicron particles involves the deterministic terms resulting from the aerodynamic convection and/or electrostatic attraction, and the stochastic term from the thermal displacement of particles. The Langevin equation describes such behavior. The Brownian dynamics algorithm was used for integration of the Langevin equation for the calculation of the single fiber deposition efficiency. Additionally the deterministic and stochastic of the particle motion were derived, using the Lagrangian and Eulerian approaches of particle movement and balance, for the calculation of the single fiber deposition efficiency due to both mechanisms separately. Combination of the obtained results allows us for calculation of the coupling effect of inertia and interception with the Brownian diffusion in a form of correlation. The results of calculation show that the omitting of the coupling effect of particular mechanism and using the simple additive rule for determination of the single fiber deposition efficiency introduces significant error, especially for particles with diameter below 300 nm.

Keywords: nanoparticle, Brownian dynamics, additivity, deposition mechanisms, Lagrangian and Eulerian models

1. INTRODUCTION

The collection of nanoparticles at particular stages of their production technology, air purification at the workplace and the atmosphere environment, requires an efficient separation method of particulate matter from the carrier gas.

Filtration is one of the effective methods for the removal of particles from an aerosol stream. The development in the specific fibrous structures promises the construction of highly efficient filters for the collection of nanoparticles. A properly designed filter structure defined by the filter porosity, diameters of used fibers and filter thickness requires also the knowledge of the key parameter of the process filtration i.e. efficiency of the single fiber deposition of aerosol particles. The main mechanism of deposition of submicron particles on the filter's fiber is the Brownian motion in which a particle randomly displaces in the carrier gas due to bombardment of the particle by the gas molecules. Coupling of this movement with convective displacement determined by the pressure drop forcing the aerosol flow, and/or another external force (electrostatic for example) causes the motion and deposition, in the consequence, of the nanoparticle to be very complex. The equation of particle motion, when the thermal displacement is included, becomes stochastic due to the presence of the rapidly fluctuating term of Brownian force. For the Lagrangian simulation of submicron particle

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deposition the Brownian dynamics algorithm will be used. The recognition of the essence of the matter of the particular mechanisms of deposition gives us a better understanding of the phenomena. Recent publications, regarding the nanoparticle filtration and deposition, van Gulijk et al. (2009), Huang and Tsai (2003), Regan and Raynor (2009) and Kim et al. (2009) indicate the necessity of more precised determination of particle deposition efficiency. Using of the Brownian dynamics algorithm we will emphasize how significant is an error, if the classical additive method is used for calculation of the single fiber filtration efficiency for simultaneously occurring mechanisms of particle deposition. There are different sources for determination of the coupled effect of the particular mechanism of deposition, namely particle tracking, which corresponds to the Lagrangian concept of particle motion, or the particle balance, related to the Eulerian model. The principles of both approaches will be discussed for comparison of the obtained results with those existing in the literature.

2. MODELING OF PARTICLE DEPOSITION

There are two major descriptions of the nanoparticle movement: Lagrangian and Eulerian. Continuum density $\rho(X,t)$ and velocity $U(X,t)$ are Eulerian fields and they are indexed by the position X in an inertial frame. Lagrangian fields are indexed by the position at reference time t_0 . The common root for both descriptions in the case of analysis of the behavior of a diffusional aerosol particle within a defined region is the Langevin equation. It was originally proposed as a stochastic model for the velocity of a microscopic particle undergoing the Brownian motion. The stochastic process $\beta(t)$ generated by the Langevin equation is called the Ornstein – Uhlenbeck process (Uhlenbeck and Ornstein, 1930) and its probability density function evolves by the Fokker – Planck equation. In the terminology of stochastic processes $\beta(t)$ is a diffusion process, and the Langevin equation is a stochastic differential equation. Let us consider the relationship between Lagrangian and Eulerian models, using the nanoparticles deposition process as an example.

2.1. Single particle trajectory concept (Lagrangian approach)

The object of our observation is the aerosol particle of diameter d_p and density ρ , entering a compartment of arbitrary shape at position X_0 (Fig. 1). The flow field within the compartment is given by vector U , and the particle has velocity V . According to Newton’s law, particle motion is described by:

$$Stk \frac{dV}{dt} = U - V + F(X,t) + A(t) \quad (1)$$

Where velocities U and V are related to average gas velocity U_0 , and time t is related to the characteristic time of the process.

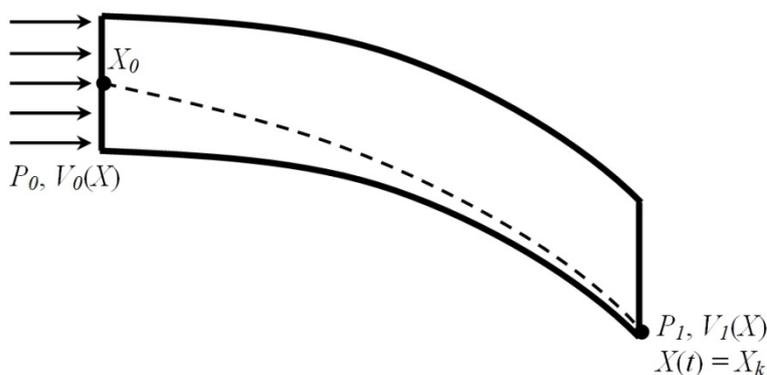


Fig. 1. Limiting trajectory of aerosol particle in the arbitrary compartment

The first term on the right side of Eq. 1 ($U-V$) represents interaction between the particle and surrounding fluid, which is assumed to be governed by Stokes' law. Stk is Stokes number, and $F(X,t)$ is an external force acting on the particle (gravity, electrostatic, etc.). Another force $A(t)$ acting on the particle is the result of collisions with molecules of the surrounding gas. $F(X,t)$ and $A(t)$ are both in a dimensionless form. These collisions make momentary changes of particle acceleration and $A(t)$ has a random pattern with respect to its quantity and direction. The following principal assumptions are made for the fluctuating part $A(t)$:

- $A(t)$ is statistically independent of $V(t)$,
- $A(t)$ varies extremely rapidly in comparison with the variation of $V(t)$,
- average in time of $V(t)$ is zero.

The second assumption implies that time intervals of duration Δt are such that during Δt the variations of V expected are very small indeed, while during the same interval $A(t)$ may undergo several fluctuations. No correlation between $A(t)$ and $A(t + \Delta t)$ exists. Equation (1) in its general form is stochastic and describes the Brownian motion of an aerosol particle. It is called the Langevin equation in its general form (Schuss 1980).

When the external force field $F(X,t)$ does not exist or can be neglected in comparison to other effects, and gas molecules are in a state of disordered motion because of disappearing forced convective diffusion, particles interact with the surrounding fluid being in a chaotic state on molecular or turbulent levels. For the first case, the Brownian displacement of a particle is the predominant mechanism of particle motion. When the fluid is in turbulent disorder, the displacement of a particle also has a random form difficult to describe in terms of particle trajectory. The interaction of particles with the complex structure of an eddy (fluid particles) of different morphology could be rather described in the form of a population balance. When the fluctuation of aerosol particles caused by thermal interaction with surrounding molecules has significant influence on the displacement, the process of particle motion is a stochastic one. A Langevin equation, which describes the motion of Brownian particles, has two terms: deterministic, representing an interaction of particle with surrounding fluid, aV , and fluctuating $A(t)$:

$$\frac{dV}{dt} = -aV + A(t) \quad (2)$$

But "solving" a stochastic differential equation like Eq. 2 differs from the ordinary procedure of solving a deterministic differential equation. It has to be understood rather in the sense of specifying probability distribution $p(V,t,V_0)$ which describes the probability that velocity has value V at time t , assuming $V = V_0$ at $t = 0$. The function p has the following properties:

$$p(V,t,V_0) \rightarrow \delta(V - V_0) \text{ when } t \rightarrow 0 \quad (3)$$

where δ is Dirac's function, and $p(V,t,V_0)$ tends to Maxwellian distribution for temperature T of the surrounding fluid, independently of V_0 as $t \rightarrow \infty$:

$$p(V,t,V_0) \rightarrow \left(\frac{m}{2\pi k_B T} \right)^{\frac{3}{2}} \exp \left(\frac{-m|V|^2}{2k_B T} \right) \quad (4)$$

where m is particle mass and k is the Boltzmann constant. The position of a Brownian particle is given in the form:

$$X(t) = X_0 e^{at} + \int_0^t e^{\beta(t,s)} A(s) ds \quad (5)$$

The integral in expression Eq. 5 can be calculated as the stochastic integral in the sense of Ito (Schuss, 1980). The construction of such an integral is a complex procedure so more useful practically as the

integration of Eq. 5 is using the Monte Carlo simulation. This procedure is simple and well described in the literature, (Kalos and Whitlock 2008). More interesting and important is another property of Brownian particle motion described by the Langevin equation. Displacements of a particle obtained from the Langevin equation form Markov's process, which is analogous to the diffusion process, (Gradoń and Podgórski, 1996, Marijnissen and Gradoń, 2010). For that process the probability distribution function $p(V, t, V_0)$ satisfies the Fokker – Planck equation. The evolution of density, σ , of system particles is defined in classical mechanics by the Liouville equation:

$$\frac{\delta \sigma}{\delta t} = \frac{\partial H}{\partial p} \frac{\partial \sigma}{\partial q} - \frac{\partial H}{\partial q} \frac{\partial \sigma}{\partial p} \quad (6)$$

where H is the Hamiltonian of the system (entire energy of the system) and p and q are generalized coordinates of the position and momentum of the system, respectively. If random effects are introduced into the system, then density σ is described by the generalized Liouville equation, called the Fokker – Planck or prospective Kolmogoroff equation written in the form of evolution of the transition probability $p(s, x, t, y)$, which is the probability of the event that the system being at time s in x will be in time t in y :

$$\frac{\delta p}{\delta t} + \frac{\partial(a(y, t)p)}{\partial y} - \frac{1}{2} \frac{\partial^2(b(y, t)p)}{\partial y^2} = 0 \quad p \rightarrow \delta(x - y) \text{ if } t \rightarrow s \quad (7)$$

where $a(y, t)$ is the deterministic drift of particles in the system and $\frac{b(y, t)}{2}$ is the diffusion coefficient (in the probabilistic sense).

If we are interested in the distribution of Brownian particles for time intervals Δt , very large in comparison with the time of particle relaxation $\tau = \frac{\rho_p d_p^2 C_C}{18\mu}$, $\Delta t \gg \tau$, then using the analogy of derivation of the Fokker–Planck equation, we receive the diffusion equation (Eq. 8).

2.2. Eulerian approach

With this path of transformations we came to the deterministic equation describing diffusional particle population balance i.e. the Eulerian approach of a model. The balance equation within a controlled differential space has the following form in the dimensionless coordinate system:

$$\frac{1}{Fo} \frac{\partial C}{\partial t} + Pe \nabla C - \nabla^2 C + B = 0 \quad (8)$$

where t is reduced time with respect to the characteristic time of the process and the space coordinates are normalized with respect to the characteristic cross-sectional dimension of compartment d , Fourier number $Fo = \frac{D \cdot T}{d^2}$, Peclet number $Pe = \frac{V \cdot d}{D}$, and $D = \frac{k_B T C_C}{3\pi\mu d_p}$ is the diffusional coefficient of a Brownian particle. C means particle concentration resulting from the integral of a particles probability distribution over the particle velocity space. Thus C means the number of particles in the control space volume at moment t . The first term in Eq. 8. means the accumulation of particles of a given size. The second term means the net transport of particles caused by the ordering effects of forced convection (or other acceleration field). The third term means the dispersion of particles due to Brownian and/or turbulent diffusion and the fourth term means the sink of particles due to their deposition or due to changes in their size caused by coagulation, evaporation or chemical reaction with surrounding gas. The last term for the deposition process can be expressed as:

$$B = \frac{1}{r_p} \left(Pe V_n C - \frac{\partial C}{\partial n} \right) \quad (9)$$

where r_p – particle diameter, V_n – velocity component of a particle normal to the surface deposition, n – direction normal to the surface of deposition.

The integration of Eq. 8 with appropriate boundary and initial conditions gives us the possibility of balancing particles within considered compartments and then calculating the efficiency of deposition.

3. THE COUPLING OF DETERMINISTIC AND STOCHASTIC MECHANISMS

The fibrous filter performance i.e. its separation efficiency and the resistance for an aerosol flow is determined by the fiber diameter distribution within the filter media of given thickness and also by the packing density of fibers. The efficiency of filtration is strongly influenced by the single fiber efficiency, E . The efficiency of particle collection depends on particle properties, flow condition and the carrier gas temperature. The main mechanisms of submicron particle deposition on the fiber are interception, inertia, convective diffusion and electrostatic attraction.

The fiber-in-cell model is frequently used for the determination of the deposition efficiency, E . For the most popular, Kuwabara model, the unit cell is a cylinder of radius R_K , coaxial with the fiber. In this geometry our simulations are realized.

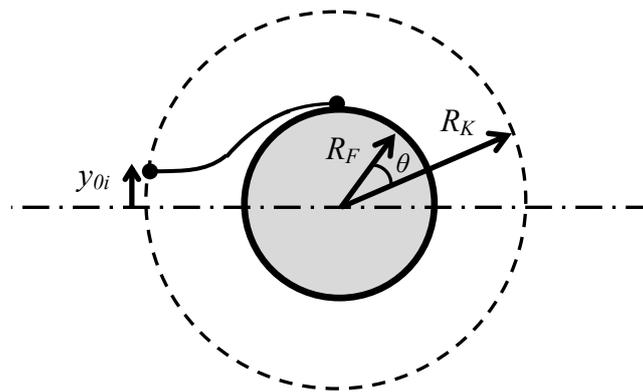


Fig. 2. Limiting particle trajectory in the Kuwabara cell

The single fiber deposition efficiency was simulated using the Brownian dynamics algorithm derived by Podgorski (2002) derived from Chandrasekhar’s (1943) method. The integration of Eq. (1) yields to normal bivariate probability distribution $\varphi_i(\Delta v_i, \Delta L_i)$ that during time interval Δt the particle will experience the change of its i^{th} component of velocity by Δv_i and it will travel the distance ΔL_i in i^{th} direction, so we can calculate the expected values $\langle \Delta v_i \rangle$, $\langle \Delta L_i \rangle$ and standard deviations σ_{v_i} , σ_{L_i} as well as coefficient of correlation ρ_{ci} . Next we generate two independent random numbers G_{L_i} , G_{v_i} , both having Gaussian distribution with zero mean and unit variance. Finally we calculate Δv_i and ΔL_i :

$$\Delta v_i = \langle \Delta v_i \rangle + G_{v_i} \sigma_{v_i} \tag{10}$$

$$\Delta L_i = \langle \Delta L_i \rangle + \rho_{ci} G_{v_i} \sigma_{L_i} + \sqrt{1 - \rho_{ci}^2} G_{L_i} \sigma_{L_i} \tag{11}$$

The detailed derivation of Eq. (10) - (11) as well as formulas for the probability distribution functions, expected values and coefficient of correlation were described by Podgórski (2002).

The algorithm described above allows particle motion to be studied accounting simultaneously for coupling between the Brownian random walk, particle inertia, convection in a moving fluid and external forces.

Firstly, the entire inlet to the Kuwabara cell was divided into 40 subintervals of the same height. From each subinterval 40 particles were released and solving the Langevin equation (Eq. 1), their random trajectory was traced. The location of the starting particle at the inlet to the Kuwabara cell above, for which no deposition on the fiber occurred, was determined. This point, y_{0cr} , defined the new height of the entrance window, which afterwards was enlarged 2.5 times, y_{0max} . The calculations were now made only for that part of the inlet to the Kuwabara cell. New 40 subintervals, i , were set and 500 particles, N_{GEN} , were released from each one. Their random trajectory was traced and the number of particles deposited on the fiber, N_{DEPi} , was counted. Then, the deposition probability, P_{Di} , as a function of the initial particle position was calculated:

$$P_{Di}(y_{oi}) = \frac{N_{DEPi}}{N_{GEN}} \quad (12)$$

The calculations were accepted only if the deposition probability was zero for at least three points located most distantly from the stagnation line $y_0 = 0$. Otherwise, the height of the entrance control window was increased to assure that the deposition probability for particles entering the Kuwabara cell above y_{0max} was really negligible. Having the final $P_{Di}(y_{oi})$ determined, the cell deposition efficiency was calculated as:

$$E_{cell} = \frac{\int_0^{R_k} P_{Di}(y_{oi}) dy_0}{R_k} \quad (13)$$

where $R_K = \frac{R_F}{\alpha^{0.5}}$ is the radius of the Kuwabara cell, R_F is the fiber radius and α is the filter packing density. Finally, the single fiber deposition efficiency, E , was determined using previously calculated cell deposition efficiency, E_{cell} , as:

$$E = \frac{E_{cell} R_K}{R_F} \quad (14)$$

Such simulations were repeated 10 times and the average efficiency was calculated.

The single fiber efficiency of deposition due to only deterministic movement was simulated using the limiting trajectory concept. The major idea of it was to examine the individual particle trajectory, contrary to the above mentioned Brownian dynamics algorithm. The equation that was solved to obtain the trajectory was the Lagrangian equation of motion (Eq. 1), neglecting the stochastic force $A(t)$ acting on the particle as the result of collisions with molecules of the surrounding gas. The starting point of the particle, y_{0cr} , was initially equal to double the fiber diameter and then decreased if the deposition did not occur. For the definitive starting location y_{oi} the single fiber collection efficiency due to deterministic mechanism, E_D , was calculated as follows:

$$E_D = \frac{y_{oi}}{R_F} \quad (15)$$

According to the Eq. 15, the E_D includes the effect of inertia and interception through the definition of the boundary condition for calculation of the particle limiting trajectory.

The single fiber efficiency of deposition due to only stochastic movement was determined by solving Eulerian equation of motion (Eq. 8) for a weightless particle using the second order upwind scheme method. Boundary conditions were assumed to be:

- dimensionless concentration was equal to zero on the fiber surface,
- dimensionless concentration was equal to one on the entrance to the Kuwabara cell.

Based on the received concentration distribution, the concentration gradient on the fiber surface $\left(\frac{dC}{dr}\right)_{r=R_F}$ was calculated and finally the single fiber collection efficiency due to Brownian movement:

$$E_B = \frac{\int_0^{2\pi} -D \left(\frac{dc}{dr}\right)_{r=R_F} R_F d\theta}{U_0 C_0 R_F} \quad (16)$$

where D is coefficient of Brownian diffusion, U_0 superficial gas velocity and C_0 concentration on the entrance to the Kuwabara cell.

4. THE COUPLING OF DETERMINISTIC AND STOCHASTIC MECHANISMS OF PARTICLE DEPOSITION. CALCULATION OF THE CORRECTION TERM.

As an example of the process analysis, the presented computations for illustration of the problem were performed for the following physiochemical and operational conditions of the process:

- properties of the filter: filter packing density $\alpha = 0.01$,
fiber radius $R_F = 5 \mu\text{m}$,
- properties of the gas: superficial gas velocity $U_0 = 0.2 \frac{\text{m}}{\text{s}}$,
density $\rho = 1.203 \frac{\text{kg}}{\text{m}^3}$,
viscosity $\mu = 1.83 \cdot 10^{-5} \text{ Pas}$,
temperature $T = 298 \text{ K}$,
mean free path $\lambda_G = 62 \cdot 10^{-9} \text{ m}$,
- the spherical aerosol particle of density $\rho_P = 1000 \frac{\text{kg}}{\text{m}^3}$,
- deposition occurs when the particle was not further than $4 \cdot 10^{-10} \text{ m}$ from the fiber,
- the time step was fixed for all particle diameters and was equal to $5 \cdot 10^{-7} \text{ s}$,
- particle diameter range from 20 nm to 900 nm.

The term defining the coupling of deterministic and stochastic mechanisms, E_{DB} , was determined using a simple rule for determination of the single fiber deposition efficiency:

$$E = 1 - (1 - E_D)(1 - E_B) \quad (17)$$

$$E = E_D + E_B + E_{DB} \quad (18)$$

Fig. 3 represents an example of calculation of the deposition efficiencies for particular effects of deposition. Calculations were performed for $R_F = 5 \mu\text{m}$ and $\alpha = 0.01$. Discrepancies between values of E and $E_D + E_B$ become significant for particles with diameters $d_p < 0.3 \mu\text{m}$. This effect is confirmed in our calculations for the range of Reynolds number $Re = \frac{2U_0 R_F \rho}{\mu} < 1$ (Stokes regime).

The single fiber collection efficiency, E , calculated assuming that all mechanisms act independently, should be equal to the single fiber collection efficiency obtained from the Eq. 14. Hence, the correlation representing the coupling of stochastic and deterministic movement was determined as follows:

$$E_{DB} = E - (E_D + E_B) \quad (19)$$

For the calculation of the deposition of nanoparticles for wide range of their diameters, the coupling term of single fiber efficiency, E_{DB} , can be determined in the form of useful correlation. The correlation involves three dimensionless numbers that emphasize the deposition mechanisms, namely Stokes number $Stk = \frac{U_0 d_p^2 \rho_P C_C}{18 \mu d_F}$ for inertial movement, Peclet number $Pe = \frac{U_0 d_F}{D}$ which means the ratio of

convective and diffusional motion of particle, and interception parameter NR that is the ratio of particle and fiber diameter. The correlation in its more general form should include the Kuwabara number which is defined by the packing density of fibers α in the filter, $Ku = -0.5 \ln \alpha + \alpha - 0.25\alpha^2 - 0.75$. It has a meaning of the scaling parameter of the gas velocity in the definition of the Pe . Formally the Kuwabara number does not change the functional form of the correlation. Results of calculation of E_{DB} for conditions defined above, Eq. 19, are shown in Fig. 4. The values of E_{DB} are shown as a function of Peclet number, Pe , and interception parameter, NR , for three different values of Stokes number, Stk , that correspond to the particles diameter of 100, 300 and 900 nm. The correlation that is valid for the wide range of Pe and the interception parameter has the following form:

$$E_{DB} = \frac{-0.909Stk^{0.255}}{Pe^{0.648}NR^{0.58}} \quad (20)$$

A similar correlation was reported by Hinds (1993) and Davies (1973).

$$E_{DB} = \frac{-1.24NR^{\frac{2}{3}}}{(Ku \cdot Pe)^{\frac{1}{2}}} \quad (21)$$

The mentioned correlation was derived from the simplified particle balance equation. The empirical formula was fitted to the curves which broke the numerical solution down into three terms: the efficiency of deposition due to diffusion, and interception with extraction of the term of combination of both mechanisms.

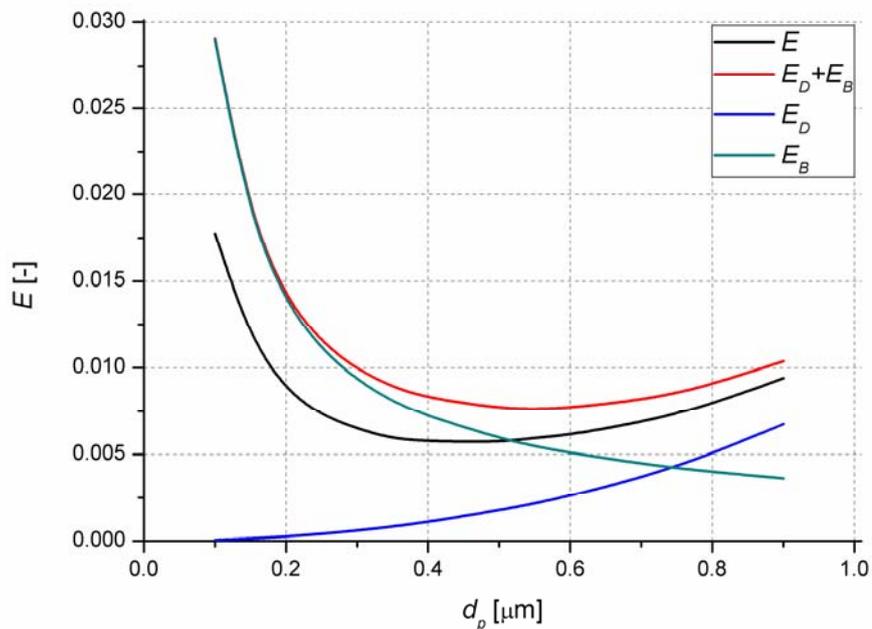


Fig. 3. Contribution of particular effects of single fiber particle deposition efficiencies, E – overall efficiency, E_D – deterministic efficiency, E_B – Brownian efficiency

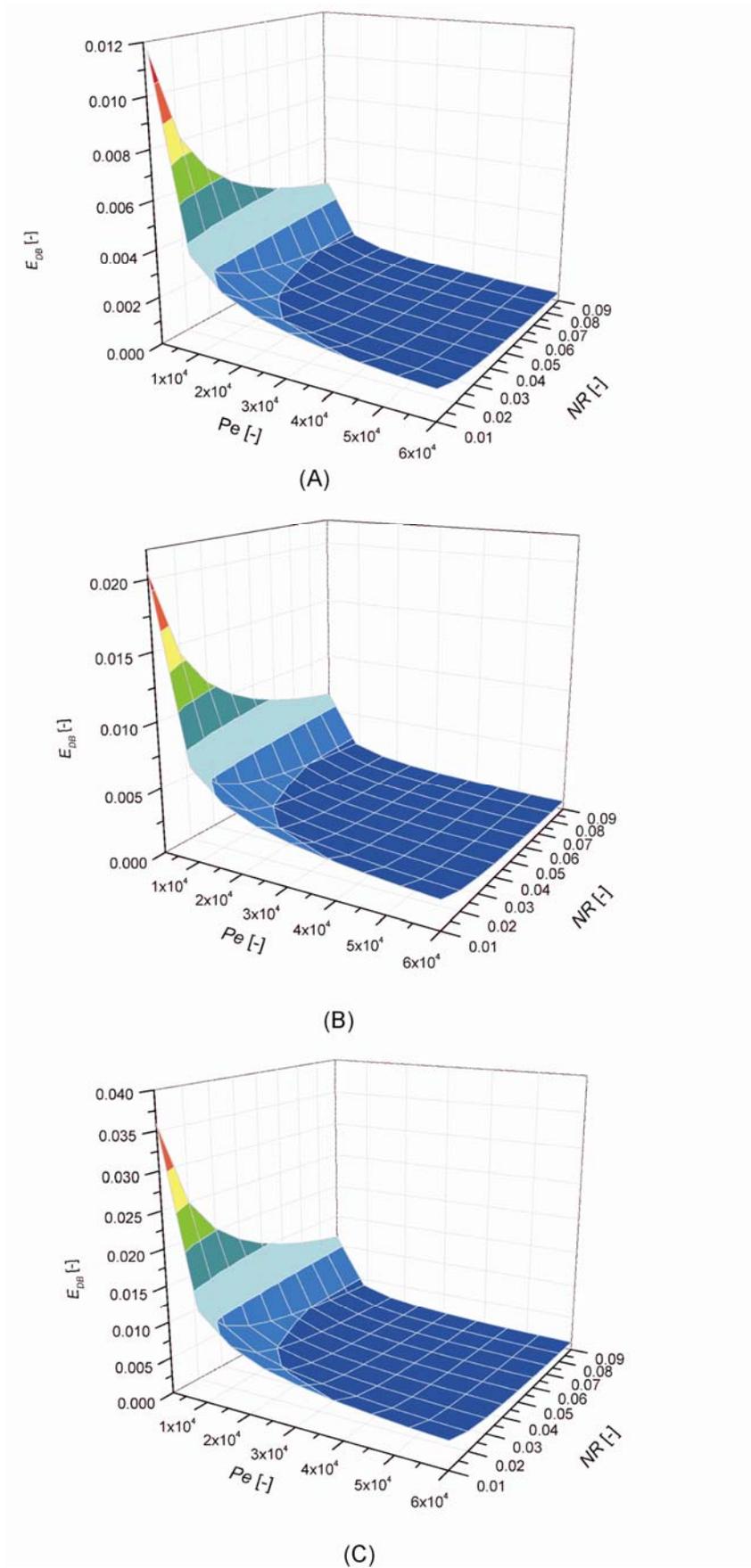


Fig. 4. Effect of the Peclet number and the interception parameter on the correlation representing the coupling of deterministic and stochastic mechanism for three different values of Stokes number.

A) $Stk=6.072 \cdot 10^{-4}$, B) $Stk=5.464 \cdot 10^{-3}$, C) $Stk=4.918 \cdot 10^{-2}$

5. CONCLUSIONS

The direct comparison of single fiber efficiencies calculated with the additive rule and with the regarding of the coupling effect is shown in Fig. 5. The data ensures that indeed, the simple, additive method of calculating the single fiber efficiency overestimates the real values. Subtracting the value of the correction term, E_{DB} , obtained from the Brownian dynamics algorithm, from the algebraic sum of E_D and E_B approaches the value E to reality. As it was shown, the effect of coupling of stochastic and deterministic mechanisms of deposition is important for nanoparticles in particular. The modeling of fibrous filters, for which the single fiber deposition efficiency E is a crucial parameter, should take this fact into account. At this point, we should mention that the calculated correlation (Eq. 20) is valid for relatively porous filters ($\alpha < 0.05$). It is the result of the assumption of the Kuwabara cell model used for our correlation. Filters with lower porosity (higher packing density of fiber) require another model of a multi-fiber system. Their essence is that the fluid in a proximity to a fiber embedded in a porous media experiences a damping body force in addition to viscous and pressure forces.

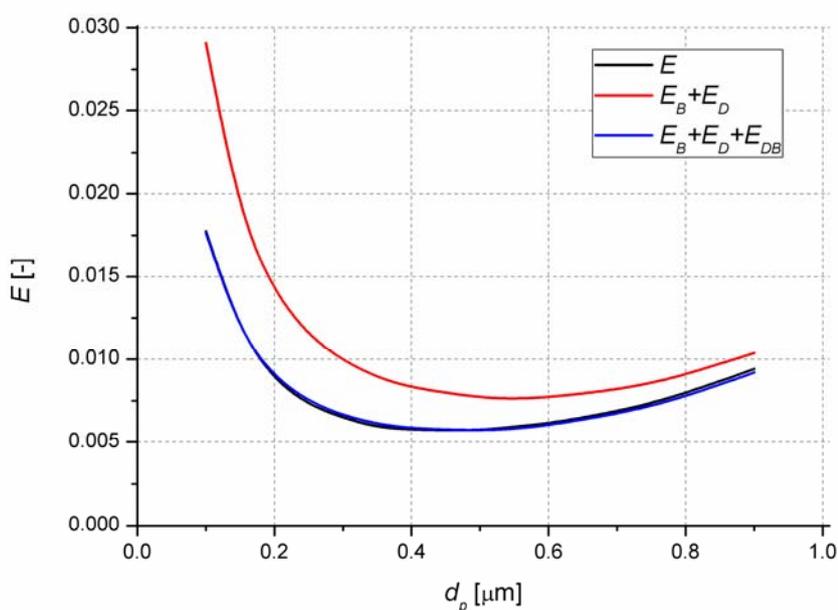


Fig. 5. Comparison of single fiber deposition efficiencies for additive rule of calculation and for consideration of the coupling effect

The improved formulae of E_{DB} (Eq. 20) obtained from fundamental theory, comparing to the only existing, experimental one (Eq. 21), correctly decreases the overall single fiber efficiency with respect to the fact that the capture of some particles might be calculated twice due to the action of different forces. It also contains the Stokes number, which introduces to the correlation the third main deposition mechanism, inertia.

Furthermore, with the increase of the particle diameter the value of E_{DB} decreases. The influence of coupling of deterministic and stochastic mechanisms tends to zero what proves the fact that the Brownian motion applies only to the small aerosol particles. Deterministic mechanisms concerns just larger ones and the correction (Eq. 20) is not necessary. The proposed correction could be useful for a quick estimation of the single fiber deposition efficiency of nanoparticles. It could be easy extend for the presence of the electrostatic effect of particle displacement combined with the aerodynamical convection and diffusion.

This work was supported by the grant ERA-NET/MNT/NFSM/1/2011.

SYMBOLS

a	deterministic drift of particles, $\text{m}\cdot\text{s}^{-1}$
A	Brownian force, N
b	double value of the diffusion coefficient (in the probabilistic sense), $\text{m}^2\cdot\text{s}^{-1}$
C	Aerosol concentration, volume fraction
Cc	Cunningham correction factor, dimensionless
D	Brownian diffusion coefficient, $\text{m}^2\cdot\text{s}^{-1}$
d_p	particle diameter, m
E	single fibre efficiency, dimensionless
E_{cell}	single cell deposition efficiency, dimensionless
E_D	single fibre efficiency due to deterministic mechanisms of deposition, dimensionless
E_B	single fibre efficiency due to stochastic mechanism of deposition, dimensionless
E_{DB}	conjugation term of single fiber efficiency, dimensionless
F	external force, N
Fo	Fourier number, dimensionless
k_B	Boltzmann constant, $\text{J}\cdot\text{K}^{-1}$
Ku	Kuwabara number, dimensionless
G_{vi}, G_{Li}	random Gaussian deviates with zero-mean and unit variance, dimensionless
ΔL_i	linear displacement along i^{th} co-ordinate, m
m	particle mass, kg
n	co-ordinate in the direction normal to the surface of deposition, m
N	number of particles, dimensionless
NR	interception parameter, dimensionless
p	transition probability, dimensionless
P_D	deposition probability, dimensionless
Pe	Peclet number, dimensionless
R_F	fibre radius, m
r_p	aerosol particle radius, m
Stk	Stokes number, dimensionless
t	time, s
T	absolute temperature, K
U	mean gas velocity, $\text{m}\cdot\text{s}^{-1}$
U_0	superficial gas velocity, $\text{m}\cdot\text{s}^{-1}$
V	particle velocity, $\text{m}\cdot\text{s}^{-1}$
x, y	Cartesian co-ordinates, m

Greek symbols

α	filter packing density, dimensionless
β	probability density function, dimensionless
λ_G	gas mean free path, m
μ	gas viscosity, $\text{Pa}\cdot\text{s}$
ρ	gas density, $\text{kg}\cdot\text{m}^{-3}$
ρ_{ci}	correlation coefficients of bivariate Gaussian distributions, dimensionless
ρ_p	aerosol particle density, $\text{kg}\cdot\text{m}^{-3}$
σ	density of particles of Hamiltonian system, dimensionless
σ_{Li}	standard deviation of the distribution of random Brownian displacements, m
σ_{vi}	standard deviation of the distribution of random velocity, $\text{m}\cdot\text{s}^{-1}$
τ	particle relaxation time, s

REFERENCES

- Chandrasekhar S., 1943. Stochastic problems in physics and astronomy. *Rev. Mod. Phys.*, 15, 1-89. DOI: 10.1103/RevModPhys.15.1
- Davies C.N., 1973. *Air Filtration*. Academic Press, London.
- Gradoń L., Podgórski A., 1996. Deposition of inhaled particles. Discussion of present modeling techniques. *J. Aerosol Med.*, 9, 343-355. DOI: 10.1089/jam.1996.9.343.
- Hinds W.C., 1999. *Aerosol Technology*. John Wiley & Sons, New York.
- Huang Ch., Tsai Ch., 2003. Mechanism of particle impaction and filtration by the dry porous metal substrates of an inertial impactor. *Aerosol Sci. Technol.*, 37, 486-493. DOI: 10.1080/02786820300968.
- Kalos M.H., Whitlock P.A., 2008. *Monte Carlo Method*. Wiley-VCH Verlag, Weinheim.
- Kim S.C., Wang J., Emery M.S., Shin W.G., Mulholland G.W., Pui D.Y.H., 2009. Structural property effect of nanoparticle agglomerates on particle penetration through fibrous filter, *Aerosol Sci. Technol.*, 43, 344-355. DOI: 10.1080/02786820802653763.
- Kuwabara S., 1959. The forces experienced by randomly distributed parallel circular cylinders or spheres in a viscous flow at small Reynolds numbers. *J. Phys. Soc. Japan*, 14, 527-532. DOI: 10.1143/JPSJ.14.527.
- Marjinissen J., Gradoń L. (Eds.), 2010. *Nanoparticles in medicine and environment*. Springer, Heidelberg.
- Podgórski A., 2002. *On the transport, deposition and filtration of aerosol particles: selected problems*, Oficyna Wydawnicza PW, Warszawa.
- Regan B.D., Raynor P.C., 2009. Single-fiber diffusion efficiency for elliptical fibers, *Aerosol Sci. Technol.*, 43, 533-543. DOI: 10.1080/02786820902777215.
- Schuss Z., 1980. *Theory and application of stochastic differential equations*. John Wiley & Sons Inc., New York.
- Van Gulijk C, Bal E., Schmidt-Ott A., 2009. Experimental evidence of reduced sticking of nanoparticles on a metal grid. *J. Aerosol Sci.*, 40, 362-369. DOI: 10.1016/j.jaerosci.2008.12.005.
- Uhlenbeck G.E., Ornstein L.S., 1930. On the theory of Brownian motion, *Phys. Rev.*, 36, 823-841. DOI: 10.1103/PhysRev.36.823.

Received 04 March 2012

Received in revised form 11 June 2012

Accepted 13 June 2012