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BROWNIAN MOTION AND THE DRIFT OF CHARGED NANOPARTICLES IN LAMINAR GAS FLOW IN A PLANE CHANNEL

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Using two limiting cases (of adsorbing and reflecting channel walls), the influence of Brownian motion on the motion of nanoparticles in laminar gas flow under the action of an external electric field has been considered. Similarity criteria making it possible to classify experimental situations have been found. Numerical modeling of deposition from the flow has been carried out with the example of the motion of a monodisperse ensemble of spherical nanoparticles with a radius of 3 nm.

Keywords: *mobility of a nanoparticle, conductivity of the wall, Galerkin method.*

Introduction. The channel motion of nanoparticles in the gas phase is widely met in new fields of technology that are related to the production of nanoparticles and their transportation, including deposition on different substrates [1–3]. An important feature of such problems is the necessity of allowing for Brownian nanoparticle motion. Analysis of effects related to the motion of nanoparticles in narrow channels is becoming increasingly important from the viewpoint of medicine, since it involves the ensurance of safe working conditions for persons working with nanoparticles [1].

This work seeks to investigate, by numerical-modeling methods, the motion of an ensemble of equally charged nanoparticles in the laminar gas flow in a plane channel under the action of an electric field and Brownian motion. We will assume that voltage U is applied to the plane-channel walls; the electric field inside the channel may be assumed to be homogeneous with a good degree of accuracy. The numerical calculations given below have been carried out under the assumption that the nanoparticles have a single charge. The external field makes it possible to efficiently control the spatial position of the ensemble of nanoparticles.

An important methodological feature of the problem in question is that the motion of the gas flow is described in the continuum approximation, whereas the mobility and the Brownian-diffusion coefficient of a nanoparticle are calculated in the free-molecular approximation. In other words, the nanoparticle radius R is fairly small, so that the Knudsen number is

$$\mathrm{Kn} = \frac{\lambda}{R} >> 1 , \tag{1}$$

where λ is the mean free path of gas molecules. In the case of atmospheric-pressure gas flow, condition (1) means that 1 nm $< R <$ 0.1 μm. Also, we use below the terminology taken earlier in describing the interaction of the gas-phase molecules with the wall, namely, we consider the adsorbing and reflecting walls separately.

Mathematical Model. Let us introduce a coordinate system: the z axis is directed along the channel axis in the direction of flow, the origin of coordinate is on the axis, too, and the y axis is perpendicular to the channel walls. In the stationary case the equation for the number density of nanoparticles $n(z, y)$ has the form

$$u(y)\frac{\partial n(z, y)}{\partial z} + v\frac{\partial n(z, y)}{\partial y} = D\frac{\partial^2 n(z, y)}{\partial y^2} , \tag{2}$$

where the parabolic profile of the gas velocity [4] is

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$$u(y) = 1.5u_0\left[1 - (2y/d)^2\right], \tag{3}$$

where u_0 is the average gas-flow velocity. The quasiequilibrium solution of Eq. (2) $n_e(y)$ has, as is easily shown, the following form:

$$n_e(y) = C\exp\left(-\frac{vy}{D}\right),$$

where C is the normalization constant. The characteristic height of the equilibrium distribution y^* is equal to $y^* = D/v$. Any nanoparticle distribution over the cross section will tend to the equilibrium distribution $n_e(y)$ for a sufficient channel length unless there are barriers to the establishment of this distribution. One of these barriers is the interaction of the nanoparticles with the wall, as will be shown below.

The velocity of a nanoparticle and the Brownian-diffusion coefficient will be determined in terms of the mobility b of the nanoparticle [5]:

$$v = beU/d, \tag{4}$$

$$D = kTb. \tag{5}$$

The quasiequilibrium distribution $n_e(y)$ takes the form of a Boltzmann distribution in an electrostatic field (that is why it is pertinent to call it the quasiequilibrium distribution), and the value of the characteristic height y^* is mobility-independent and is equal to

$$y^* = d\frac{kT}{eU}.$$

Thus, for U = 10 V, $d = 10^{-2}$ m, and T = 900 K, the characteristic height is $7.8\cdot10^{-5}$ m.

According to [5], the mobility of a spherical nanoparticle in the gas flow is equal to

$$b = \frac{3}{16\pi R^2 P}\left(\frac{2\pi kT}{m}\right)^{0.5}. \tag{6}$$

Next we assume that the nanoparticle motion in a one-component gas is considered. Formulas for a mixture of gases have been given in [2].

Before we pass to numerical calculations, we evaluate the process of deposition of nanoparticles on the basis of a qualitative analysis of Eq. (2). Comparing the term on the right-hand side of (2) and the second term on the left-hand side of the equation, we can say that the influence of the Brownian motion compared to that of the electric field can be disregarded if the inequality

$$\chi = \frac{D}{vd} = \frac{kT}{Ue} << 1 \tag{7}$$

holds. In other words, the Brownian motion can be disregarded if the energy of thermal motion is much lower than the nanoparticle's kinetic energy acquired under the action of the external electric field. Comparing both terms on the left-hand side of the equation, we evaluate the path L on which the influence of the electric field can be disregarded if the inequality

$$\frac{vL}{u_0 d} = \frac{ebUL}{u_0 d^2} << 1 \tag{8}$$

holds.

The boundary conditions on the channel walls for the number density of nanoparticles n are dependent on the physics (still not clearly understood) of interaction of nanoparticles with a solid wall, primarily, on the smoothness of the wall on a nanoscale. Therefore, in what follows, we restrict ourselves to investigation of just two limiting cases: those of adsorbing and reflecting walls. In the case of the adsorbing wall we believe that any nanoparticle remains on it after touching it. Neutralization of the charge of nanoparticles that have touched the wall requires the additional assumption that the wall is metallic. For the case of the reflecting channel wall, it is believed that, even reaching it, the nanoparticles return to the gas phase. Furthermore, in this work, the reflecting wall is assumed to be dielectric, so that the nanoparticles remain charged even after contact with the wall and return to the gas phase with the same charge.

For the adsorbing wall, we have the following boundary conditions to Eq. (2):

$$\text{for any } z \quad n\left(z, \frac{d}{2}\right) = n\left(z, -\frac{d}{2}\right) = 0 . \tag{9}$$

For the reflecting wall, the boundary conditions to Eq. (2) are "nonflow" conditions:

$$vn - D\nabla n\left(z, -\frac{d}{2}\right) = vn - D\nabla n\left(z, \frac{d}{2}\right) = 0 . \tag{10}$$

Any actual walls represent a certain case intermediate between two limiting cases: of adsorbing and reflecting walls.

For the sake of simplicity, we will use the initial conditions to (2), which are consistent with boundary conditions (9) for the adsorbing wall, in the form

$$n\,(0, y) = A\cos(\pi y/d) . \tag{11}$$

Calculation Results. Application of the Galerkin Method. In considering situations where it is necessary to allow for the Brownian diffusion of nanoparticles and their drift under the action of the external electric field, we use today's version of the Galerkin method [6, 7] to obtain analytical evaluations. For the evaluations, we will seek the solution in the form

$$n\,(z, y) \simeq A\,(z)\cos(\pi y/d) \tag{12}$$

with an unknown amplitude $A(z)$. Substituting (12) into Eq. (2) and following the mathematical technique of the Galerkin method [6], we obtain the ordinary differential equation for the amplitude of the largest-scale mode (12):

$$\frac{dA\,(z)}{dz} = -A(z)\frac{\pi^2 k_1}{d^2 k_0} , \tag{13}$$

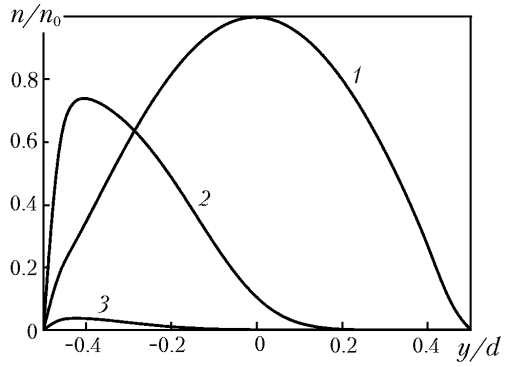
where the coefficients k_0 and k_1 have been determined as follows:

$$k_0 = 1.5u_0 \int_{-d/2}^{d/2}\left[1 - \left(\frac{2y}{d}\right)^2\right]\cos^2\left(\frac{\pi y}{d}\right)dy \approx 6.5\cdot 10^{-3}u_0 , \tag{14}$$

$$k_1 = \int_{-d/2}^{d/2}\cos^2\left(\frac{\pi y}{d}\right)dy \approx 5\cdot 10^{-3} . \tag{15}$$

The solution of (13) has the form

$$A\,(z) = A_0\exp\left[-z\frac{\pi^2 k_1 D}{d^2 k_0}\right] = A_0\exp\left[-z/l_B\right] , \tag{16}$$



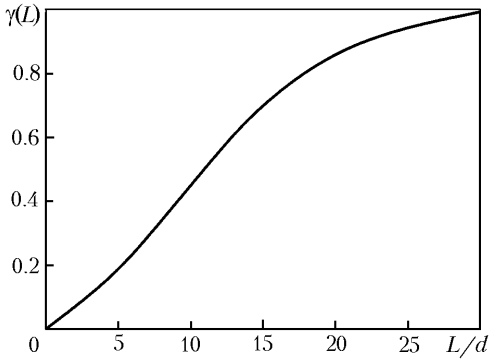


Fig. 1. Profiles of the number density of nanoparticles over the channel width: 1) z/d = 0.15, 2) 15, and 3) 30.

Fig. 2. Share of deposited nanoparticles.

which yields a formula for the characteristic Brownian-deposition length l_B:

$$l_B = \frac{d^2 k_0}{\pi^2 D k_1} \simeq \frac{d^2 u_0}{\pi^2 D}.$$

Actually, $1/l_B$ is the approximate value of the least eigenvalue of the problem in question. We emphasize that, as follows from (16), the electric field influences modes that are smaller in scale than the mode (12) in question. The first of these modes satisfying boundary conditions (9) is the mode sin $(2\pi y/d)$. The equation for the amplitude of this mode has been omitted for the sake of brevity.

The analytical expressions obtained above are useful in analyzing numerical results. In particular, for channel flow with typical parameters u_0 = 0.2 m/sec, T = 900 K, R = 3 nm, and d = 0.005 m, the characteristic length is l_B = 1.4 m. Thus, for processes on a smaller length, the role of Brownian motion is secondary in such a system.

Numerical Results. Equation (2) with boundary conditions (9) has been solved numerically in the Mathcad 2000 environment by the method of lines, which makes it possible to reduce the partial differential equation with a variable coefficient to a system of ordinary differential equations [8]. The calculation results are given below.

Figure 1 shows the change in the density of nanoparticles over the channel cross section for the channel with adsorbing walls. The electric field is directed to the wall with a coordinate $y = -0.5d$, u_0 = 0.2 m/sec, U = 10 V, and d = 0.005 m. For this example, inequality (7) holds; it is seen that at the beginning of the channel, we mainly have the displacement of the cloud of nanoparticles under the action of the electric field. At the end of the channel, the nanoparticles are still present in its central part (curve 3), since the Brownian diffusion counteracts the drift under the action of the electric field. It is noteworthy that we have the parameter $\chi \sim 0.01$ even for a low applied voltage, i.e., the Brownian diffusion of nanoparticles in this case will be important only for large gradients of their number density. In particular, the Brownian diffusion of nanoparticles participate in the formation of profile 3 in Fig. 1.

The share of nanoparticles $\gamma(L)$ deposited on the channel wall on the path L is easily computed using the expression

$$\gamma(L) = \frac{\int_0^L u(y)\,[n(0, y) - n(L, y)]\,dy}{\int_0^L u(y)\,[n(0, y)]\,dy}. \qquad (17)$$

The function $\gamma(L)$ is plotted in Fig. 2 for the same conditions as those in Fig. 1. Interestingly, the deposition density is virtually uniform on the first 20 calibers. Clearly, by decreasing voltage, we can attain the uniformity of deposition on the length $30d$, too. The deposition of nanoparticles is more rapid with increase in the voltage, all other things

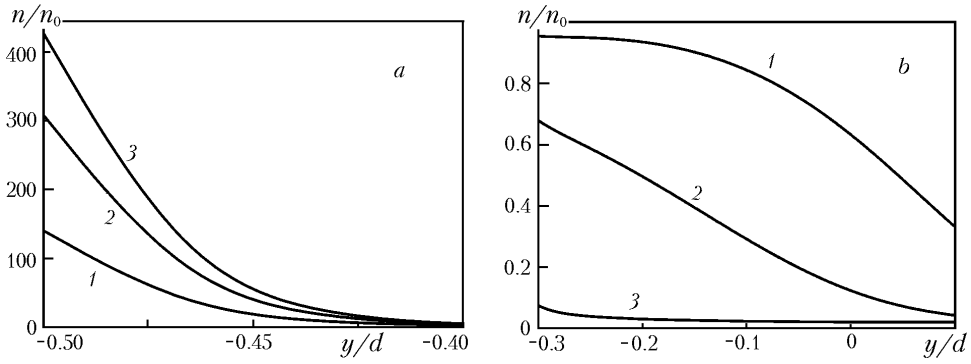


Fig. 3. Profiles of the number density of nanoparticles at the channel wall: 1) z/d = 7.5, 2) 15, and 3) 30.

being equal. As follows from the plots in Figs. 1 and 2, the Brownian diffusion reduces the efficiency of deposition under the action of the electric field.

Figure 3a shows the evolution of the nanoparticle-density distribution over the cross section for the channel with reflecting walls. It is seen that as the cloud moves in the channel, the density of nanoparticles at the wall toward which the external field pushes them, increases. The formation of the exponential profile is seen. We assume that the nanoparticles do not lose their charge as a result of contact with the wall and the adhesive forces are fairly small. Also, we disregard the mutual repulsion of charged nanoparticles in this work, assuming their density to be fairly low. We emphasize that the quasiequilibrium distribution of nanoparticles $n_e(y)$ is yet to be attained even for curve 3 in Fig. 3a. For this curve, virtually all nanoparticles are in the 10% zone of the channel width. It is noteworthy that in the central part of the channel, curve 1 lies much higher than curves 2 and 3. The nanoparticle distribution in this part of the cross section is shown in Fig. 3b.

In motion of uncharged particles in the channel with reflecting walls, a virtually uniform nanoparticle distribution over the channel cross section would be attained due to the Brownian diffusion on lengths comparable to l_B.

To compute the drift velocity of nanoparticles from formula (4) it is necessary that the strength of the electric field E_1 produced by the charged nanoparticles be much lower than the strength of the electric field. One Maxwell equation [8] yields the relation between E_1 and $n(z, y)$:

$$\nabla \cdot E_1 = en/\varepsilon_0 , \tag{18}$$

where ε_0 is the permittivity of free space. Expression (18) yields the approximate relationship

$$n \approx \frac{E_1 \varepsilon_0}{de} ,$$

as a result we have the inequality

$$n << \frac{U\varepsilon_0}{d^2 e} . \tag{19}$$

In particular, for U = 10 V and d = 0.005 m, we obtain from inequality (19) that the number density of nanoparticles is $n << 10^{13}$ m^{-3}.

Conclusions. We have carried out the theoretical and computational investigation of the motion of charged nanoparticles in a plane channel in the presence of a constant external electric field. The criteria of influence of the Brownian motion of nanoparticles on their distribution in the channel have been determined. The results of the qualitative analysis have been supplemented with the data of numerical calculations for spherical nanoparticles with a radius of 3 nm. Since the coefficient of Brownian diffusion of nanoparticles in the free-molecular regime is in inverse proportion to their radius squared, the influence of the Brownian diffusion on the distribution of larger nanoparticles is

much smaller. The primary importance of the interaction of the nanoparticles with the channel walls and the influence of this interaction on the form of the nanoparticle distribution in the cross section of the channel have been shown. In the work, we have investigated two limiting cases: those of adsorbing and reflecting channel walls. Experimental results on the influence of the charged wall on the deposition of nanoparticles have been given in [9].

Physically it is clear that Brownian motion in our problem prevents the deposition of nanoparticles. Thus, reduction in the system's temperature makes it possible to increase the deposition intensity due to the decrease in the Brownian-diffusion coefficient, all other things being equal. As the gas pressure in the system decreases, the influence of the Brownian diffusion of nanoparticles grows according to formula (6).

In motion of uncharged nanoparticles in the isothermal laminar gas flow, Brownian motion is the only reason for their deposition on the walls. This deposition on the walls will be a pronounced effect only for channel lengths comparable to the characteristic length l_B [2].

Modeling of the electrodynamic focusing of charged nanoparticles at the center of the channel using a variable electric field is the subject of our investigations.

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NOTATION

A, mode amplitude, m^{-3}; D, Brownian-diffusion coefficient, m^2/sec; b, mobility of a nanoparticle, sec/kg; d, channel height, m; E, electric-field strength, V/m; e, electron charge, C; k, Boltzmann constant; Kn, Knudsen number; L, channel length, m; l_B, characteristic Brownian-deposition length, m; m, weight of a carrier-gas molecule, kg; P, pressure in the channel, Pa; R, radius of a nanoparticle; T, gas temperature, K; $u(y)$, gas-velocity profile, m/sec; U, applied voltage, V; v, drift velocity, m/sec; ε_0, permittivity of free space, F/m; χ, dimensionless parameter; λ, mean free path of gas molecules, m; γ, share of nanoparticle deposited on the walls. Subscripts; e, equilibrium.

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