

CALCULATION OF A TRANSPORT CURRENT FROM A NOZZLE WITH TWO-PHASE FLOW IN THE PRESENCE OF A CORONA DISCHARGE

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The operation of a source of charged aerosol particles which consists of a supersonic nozzle, a corona-forming needle-shaped electrode, and a device for injecting liquid droplets into a gas flow is considered. A theoretical model for two-dimensional, two-phase flow in the nozzle is considered. An algorithm of numerical calculation of such a flow is developed, and results of calculations of the electric transport current from the nozzle are given.

Introduction. In aerosols consisting of a gas, ions, and disperse-phase particles (droplets), the latter can acquire an electric charge as a result of deposition on them of ions. Since calculations of flows of charged aerosols are complicated, especially with allowance for the effect of the intrinsic electric field, this problem has been the subject of a rather small number of studies. Ushakov and Franchuk [1] studied one-dimensional flows of aerosols with allowance for migration charging of particles. In the majority of applications, however, it is necessary to take into account both the migration and diffusion electrification of particles. Vasil'eva et al. [3] studied such flows in a one-dimensional formulation using the asymptotic formulas from [2]. A much more complicated case of non-one-dimensional gas flow with dispersed particles in a Laval nozzle is considered below. Two-dimensional distributions of ion concentrations, space charge of droplets, and electric-current density, which are required to determine the transport current, are obtained for arbitrary Peclet electrical numbers Pe_E .

The goal of this work is to develop a numerical method for simulating processes in a nozzle with a corona discharge that can be used to study and optimize the source of charged aerosol.

Simulation was performed in the nozzle shown schematically in Fig. 1. The forechamber pressure is $p_0 = 0.1\text{--}1$ MPa, the temperature is $T_0 = 373$ K, and the carrier gas is air. Droplets were injected into the flow in the broad part of the nozzle (in section AA_1). The hydrodynamics of this process was not considered. It was assumed that in section AA_1 there is a uniformly distributed flow of droplets with a known concentration.

The corona-forming electrode is the needle A_1C , and the walls of the axisymmetric nozzle serve as the second electrode. Between the electrodes, external sources produce a potential difference φ_w of about 2–30 kV. The characteristic electric-field strength in the nozzle throat is $E_0 \sim 10^3$ kV/m.

Switching on the potential difference between the electrodes gives rise to a corona discharge in a neighborhood of the needle. The gas ions formed produce a space charge, which is carried by the flow containing liquid droplets. Besides the motion of the carrier gas, the ions are acted upon by the electric field. As a result, the streamlines of the ions and the carrier gas do not coincide. While moving, the ions stick to the droplets, which are assumed to move together with the carrier gas and are removed from the nozzle. The flow of charged droplets and the ion flow generate an electric transport current from the nozzle.

Construction of a Flow Model for the Flow. A model for the flow of the two-phase multicomponent mixture described above is constructed under the following assumptions.

The degree of ionization of the gas carrier in the corona discharge is considered small (about 10^{-10} , i.e., at a pressure of 101.3 kPa, the number of ions in the external area of the corona discharge is about

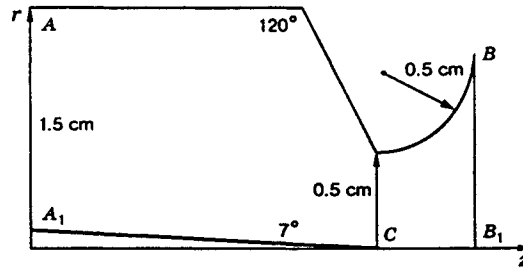


Fig. 1

10^{13} – 10^{15} m^{-3}). Therefore, the effect of the applied electric field on the motion of the carrier medium is ignored. The volume concentration of the droplets is low (of the order of 10^{-2}), and their influence on the motion of the carrier medium is also ignored.

The motion of the carrier medium (which is compressed, inviscid, and non-heat-conducting) is calculated within the framework of the theory of a Laval nozzle in a quasi-one-dimensional approximation. Particles with a characteristic size of about $(1-3) \cdot 10^{-6}$ m are considered. It is known that particles of such small sizes are frozen in the carrier medium, and high-speed slip is absent. Therefore, in a steady flow, the particles move along streamlines of the carrier medium.

The velocity of diffusion of the gas ions is determined by the Reynolds electrical number Re_q , which is equal to the ratio of the characteristic velocity of the medium to the velocity of drift of an ion in the characteristic electric field. For pressures of 0.1–1 MPa, a temperature of about 400 K, and a field strength of about 10^3 kV/m, the value of Re_q varies from 0.2 to 3. Therefore, the gas ions generally move under the action of two forces — the friction force from the carrier medium and the Coulomb force. Since the directions of the electric field and streamlines of the carrier medium do not coincide, the motion of the gas ions cannot be considered one-dimensional. To calculate the distributions of the gas-ion density in the nozzle, it is necessary to use two-dimensional equations. As a result, the density distribution of the space charge of the droplets on whose surface the gas ions are precipitated in motion is apparently also two-dimensional.

Basic Equations. The carrier medium is considered as a perfect gas. The effect of the particles and gas ions on the motion of the carrier medium is ignored. The equations of motion integrated with initial conditions corresponding to the receiver conditions (p_0 , ρ_0) have the form

$$\frac{p_0}{p} = \left(1 + \frac{\gamma - 1}{2} M^2\right)^{\gamma/(\gamma-1)}; \quad (1)$$

$$\frac{\rho_0}{\rho} = \left(1 + \frac{\gamma - 1}{2} M^2\right)^{1/(\gamma-1)}; \quad (2)$$

$$\frac{\sigma}{\sigma_{\min}} = \left(M \int_0^1 \cos \alpha(\xi) d\xi\right)^{-1} \left[\frac{2}{\gamma-1} \left(1 + \frac{\gamma-1}{2} M^2\right)^{(\gamma+1)/2(\gamma-1)}\right]. \quad (3)$$

In this case, $\alpha(\xi) = \arctan [(R_H)'_z + \xi((R_B)'_z - (R_H)'_z)]$, $\sigma = \pi R^2$, $\sigma_{\min} = \pi R_{\min}^2$, and $F'_z = dF/dz$. Here z is the coordinate along the nozzle axis, $R_B(z)$ is the distance from the nozzle axis to its walls, $R_H(z)$ is the distance from the nozzle axis to the surface of the needle, $\sigma(z)$ is the cross-sectional area of the nozzle, p is the pressure, ρ is the density, $M = \rho V^2/\gamma p$ is the current Mach number ($\gamma = c_p/c_v$), $V = (u^2 + v^2)^{1/2}$ is the modulus of the gas velocity, and u and v are the axial and radial velocity components.

Equation (3) is used to determine the Mach number M from the specified nozzle shape $R(z)$. After finding the M , we determined the pressure and density from (1) and (2) and then the modulus of the velocity of the carrier gas:

$$V = M \left(\frac{\gamma p}{\rho}\right)^{1/2}. \quad (4)$$

The velocity components u and v are calculated under the assumption that the flow is quasi-one-dimensional, and, hence, the streamlines of the carrier medium are defined by the equations

$$R(z) = R_H(z) + \xi[R_B(z) - R_H(z)],$$

where the parameter ξ varies from 0 to 1. The set of intermediate values of ξ allows the streamline shape to be gradually varied from the one close to the nozzle contour at the walls to an almost straight line near the axis.

In a cylindrical coordinate system (z, r) with the z axis along the nozzle axis (see Fig. 1), the equations describing the motion of the gas ions have the form

$$\frac{\partial q}{\partial t} + \frac{1}{r} \frac{\partial}{\partial r} (r j_r) + \frac{\partial}{\partial z} (j_z) = -w, \quad j_r = q(v + b_i E_r), \quad j_z = q(u + b_i E_z). \quad (5)$$

Here $q = en_i$ is the space-charge density of the ions, j_r and j_z are the density components of the electric current of the gas ions, n_i is the ion concentration, e is the proton charge, $b_i = eD_i/kT$ is the mobility coefficient of the ions (D_i is the diffusivity of the ions, T is the temperature, and k is the Boltzmann constant), E_r and E_z are the components of the electric-field strength, and w is the rate of sticking of the ions to the droplets

$$w = n_p J_i. \quad (6)$$

Here J_i is the gas-ion current per one particle, and n_p is the concentration of particles of radius a . It is assumed that the ions are singly charge and positive.

The equations for the electric potential φ have the form

$$\frac{\partial^2 \varphi}{\partial r^2} + \frac{1}{r} \frac{\partial \varphi}{\partial r} + \frac{\partial^2 \varphi}{\partial z^2} = -\frac{4\pi}{\epsilon} (q + q_p), \quad E_r = -\frac{\partial \varphi}{\partial r}, \quad E_z = -\frac{\partial \varphi}{\partial z}, \quad (7)$$

where ϵ is the dielectric constant of the medium, $q_p = n_p e_p$ is the space-charge density of the particles, and e_p is the particle charge. The quantity e_p is variable because the sticking of the ions proceeds throughout the residence time of the particles in the flow.

For Eq. (7), it is necessary to specify boundary conditions. On metallic surfaces: the potential difference $\varphi = \varphi_w$ on the needle and $\varphi = 0$ on the nozzle walls (the walls are grounded). At the channel entry (in section AA_1) $E_z = 0$, and at the exit from the channel (in section BB_1) $\varphi = 0$. The last condition corresponds to the assumption of a grounded grid at the nozzle cutoff with zero hydrodynamic drag force.

We formulate a boundary condition for Eq. (5) on the surface of the needle. In a corona discharge in air with almost atmospheric pressure near the surface of the corona-forming electrode, a great number of ionization and other electrokinetic processes occur. Detailed consideration of these processes is beyond the scope of the present paper. Following the well-known experimental data [4], we assume that the indicated processes take place in a rather thin boundary layer near the needle surface. On the outer boundary of the layer there is a steady flow of gas ions of identical sign with space charge density q depending on the local strength of the electric field on the needle surface and discharge parameters. Experimental studies of a corona discharge in a gas stream give an analytical relation between the electric-field strength E_w on the needle surface and the gas parameters [4]. From the values of the gas parameters in the vicinity of the needle we calculate the value of E_w , which will be used as a deficit condition to close the problem, because it is not possible to determine experimentally or theoretically the density of the space charge formed by the gas ions on the outer boundary of the corona-discharge cover. Use of E_w to close the problem in [5] by an iterative procedure makes it possible to find the ion concentration on the boundary by solution of the problem using numerical methods. The iterative procedure consists of the following. The value of the space-charge density of the ions q_w on the outer boundary of the corona cover is sought using the recursive relation

$$q_w^{(s+1)} = q_w^{(s)} \exp \left[\alpha \left(\frac{E_w^{(s)}}{E_w} - 1 \right) \right]. \quad (8)$$

Here the superscript indicates the iteration number, $E_w^{(s)}$ is the electric-field strength obtained by numerical solution of the problem in the s th iteration, and α is the damping factor (in calculations, $\alpha \sim 0.5$). The

iterations start with a solution of the problem for a certain value $q_w^{(0)}$ and are finished when the value of $E_w^{(s)}$ coincides with adequate accuracy with E_w . The formula for calculating E_w from the gas parameters and the geometrical characteristics of the electrode is given below.

Calculation of the Sticking of Ions to Droplets. According to the assumptions used, the flow region outside the corona cover contains gas ions of identical sign and aerosol particles, which are not charged when they are injected into the flow. A model for charging (electrification) of such particles in their motion in the region containing ions of identical sign (in the region of a unipolar space charge) is described below.

The unipolar charging of aerosol particles is generally described by solution of the Cauchy problem

$$\frac{de_p}{dt} = J_i, \quad t = 0: \quad e_p = 0. \quad (9)$$

In the stationary problem of the motion of particles along streamlines of the carrier medium, the derivative d/dt contains only the convective part Vd/dl , where l is the distance along a streamline.

The dependence of J_i on the flow parameters is determined by the state of the carrier gas, the dimensions and properties of the particle surface, etc. The finding of this dependence is a separate and frequently very complicated problem.

We consider the case of rather large spherical particles whose radius a far exceeds the characteristic path length of the gas ions l_i . The ion distribution in the vicinity of a particle and the electrification current J_i are found by solving the following boundary-value problem [6]:

$$\begin{aligned} \operatorname{div} \mathbf{j} = 0, \quad \mathbf{j} = -D_i \nabla q_* + q_* b_i \mathbf{E}_*, \quad r = a: \quad q_* = 0, \quad r \rightarrow \infty: \quad q_* \rightarrow q, \\ \mathbf{E}_* = -\nabla \varphi_*, \quad \varphi_* = -(\mathbf{E} \cdot \mathbf{r}) \left(1 - \frac{a^3}{r^3}\right) + e_p \left(\frac{1}{r} - \frac{1}{a}\right), \quad J_i = -\int_S j_n ds, \quad j_n = (\mathbf{j} \cdot \mathbf{n}). \end{aligned} \quad (10)$$

Here q_* and \mathbf{E}_* denote "microscopic" values of the space-charge density and the electric-field strength, which, with distance from the particle, tend to the background "macroscopic" values of q and \mathbf{E} ; \mathbf{j} is the electric-current density of the ions, φ_* is the electric-field potential, S is the surface of a particle, \mathbf{n} is the outer normal to it, and \mathbf{r} is the radius vector from the center of the particle. In writing Eq. (10) we have ignored the intrinsic electric field of the ions, the particle motion relative to the gas, and the unsteadiness of the process. Estimates show that such assumptions are true for the class of flows considered. After finding of the space-charge distribution from the solution of problem (10), the electric current on the particle surface is determined by integration.

Generally, problem (10) does not have an exact analytical solution, but its numerical [6] or approximate analytical solutions can be constructed with allowance for the small parameters: the Peclet number $\operatorname{Pe}_E = ea|E|/kT$ for $\operatorname{Pe}_E \ll 1$ and Pe_E^{-1} for $\operatorname{Pe}_E \gg 1$. Such solutions are obtained in [2, 7] by the method of matched asymptotic expansions. We use the expressions obtained in [2, 7] for the electrification current:

$$\operatorname{Pe}_E \rightarrow 0: \quad J_i = 4\pi a D_i q [I_0 + o(\operatorname{Pe}^2)], \quad I_0 = \Lambda \left[1 + \frac{1}{2} \operatorname{Pe}_E \Lambda \exp(e_p^*)\right], \quad \Lambda = e_p^* (\exp e_p^* - 1)^{-1}; \quad (11)$$

$$\operatorname{Pe}_E \rightarrow \infty: \quad J_i = 4\pi a D_i q [I_\infty(\operatorname{Pe}_E, e_p^*) + o(\operatorname{Pe}_E^{-4/3})], \quad I_\infty(\operatorname{Pe}_E, e_p^*) = 3\operatorname{Pe}_E (I_1 + \chi I_2 + \chi^{4/3} I_3). \quad (12)$$

In this case,

$$|e_p^0| \leq 1: \quad I_1 = \frac{1}{4} (1 - e_p^0)^2, \quad I_2 = \frac{1}{4} (1 - e_p^{02})^{1/2}, \quad |e_p^0| > 1: \quad I_1 = \frac{1}{2} (\operatorname{sgn} e_p^0 - 1) e_p^0, \quad I_2 = 0,$$

$$I_3 = \left\{ \frac{e_p^1}{8} \left[\exp(4.16 e_p^1) - 1 \right]^{-1} \right\}^{1/2} - f(e_p^1), \quad e_p^1 \geq 0: \quad f = 0, \quad e_p^1 < 0: \quad f = \left(\frac{|e_p^1|}{8} \right)^{1/2},$$

$$e_p^* = \frac{e_p e}{akT}, \quad e_p^0 = \frac{e_p^*}{3\operatorname{Pe}_E}, \quad e_p^1 = (|e_p^0| - 1) \chi^{-2/3}, \quad \chi = \frac{2}{3\operatorname{Pe}_E}.$$

Calculations using formulas (11) and (12) agree well with the numerical solution in [6] of problem (10). To calculate the electrification of the particles not only for the limiting but also for moderate values of Pe_E , it

is possible to use the interpolation formula derived on the basis of (11), (12), and the numerical calculations of [2]:

$$J_i^{(1)} = 4\pi a D_i q I^*. \quad (13)$$

Here $I^* = I_0(\alpha Pe_E, e_p^*)(1 - \nu) + \nu I_\infty(Pe_E, e_p^*)$, $\alpha = 1 + 2.8 Pe_E^{1.79}$, and $\nu = Pe_E^2(1 + Pe_E^2)^{-1}$.

For $Pe_E \ll 1$ and $Pe_E \gg 1$, formula (13) becomes expressions (11) and (12), respectively. Formula (13) allows one to determine the right side of Eq. (9) for flows with strong variations in the electric field, which include flows with a corona-forming electrode. Often, the condition $\lambda = l_i/a \ll 1$ used in the formulation of problem (10) is not satisfied. An example is the charging of submicron particles under atmospheric conditions. Of the considerable number of papers on particle electrification for $\lambda \gg 1$, mention should be made of the paper of White [8], in which the free-molecular motion of ions in the vicinity of a particle is considered. Without considering details of the derivation, we give the result obtained by White:

$$J_i^{(2)} = \pi a^2 v_t q \exp(-e_p^*) \quad (14)$$

(v_t is the thermal velocity of the ions). To calculate J_i in the poorly studied region $\lambda \sim 1$, it seems reasonable to use the combination

$$J_i = \tau J_i^{(1)} + (1 - \tau) J_i^{(2)}, \quad \tau = (1 + \lambda)^{-1}. \quad (15)$$

System of Equations for Calculating the Transport Current from the Nozzle. To solve the posed problem numerically, we write a system of equations in dimensionless form. For this, we introduce the following dimensionless variables:

$$\begin{aligned} p^* &= \frac{p}{p_0}, \quad \rho^* = \frac{\rho}{\rho_0}, \quad V^* = \frac{V}{u_0}, \quad u_0 = \left(\frac{p_0}{\rho_0}\right)^{1/2}, \quad q^* = \frac{q}{q_0}, \quad b^* = \frac{b}{b_0}, \\ E^* &= \frac{E}{E_0}, \quad E_0 = \frac{\varphi_w}{L}, \quad n_p^* = \frac{n_p}{n_p^0}, \quad e_p^* = \frac{e_p}{e_{p0}}, \\ J_i^* &= \frac{J_i}{4\pi a D_i q_0}, \quad \varphi^* = \frac{\varphi}{\varphi_w}, \quad e_{p0} = \frac{akT_0}{e}, \quad r = \frac{r}{L}, \quad z^* = \frac{z}{L}, \quad t^* = \frac{tu_0}{L}. \end{aligned}$$

Here p_0 , ρ_0 , and T_0 are the gas properties in the receiver, L is the radius of the cylindrical portion of the nozzle, and n_p^0 is the droplet concentration at the entry to the cylindrical part of the nozzle. The value of n_p^0 is calculated from the mass flow rate of the liquid injected into the nozzle using the formula

$$n_p^0 = \frac{G}{u_0^0 \pi L^2 (4/3) \pi a^3 \rho_w^0}.$$

Here G is mass-flow rate of the liquid, the gas velocity u_0^0 in section AA_1 (see Fig. 1) is calculated from isentropic relations with allowance for the receiver conditions, and ρ_w^0 is the density of the droplet material.

The equations of motion for the carrier medium (1)–(4) are already written in dimensionless form:

$$p^* = \left(1 + \frac{\gamma - 1}{2} M\right)^{-\gamma/(\gamma-1)}, \quad \rho^* = \left(1 + \frac{\gamma - 1}{2} M\right)^{-1/(\gamma-1)}, \quad V^* = M \left(\frac{\gamma p^*}{\rho^*}\right)^{1/2}.$$

With allowance for expressions (6) and (13), the equation of continuity of the ions (5) is written dimensionless form

$$\frac{\partial q^*}{\partial t^*} + \frac{\partial}{\partial z^*} q^* \left(u^* + \frac{b^*}{Re_q} E_z^*\right) + \frac{1}{r} \frac{\partial}{\partial r} r^* q^* \left(v^* + \frac{b^*}{Re_q} E_r^*\right) = -R_s (n_p^* q^* I^*). \quad (16)$$

Expression (16) contains two dimensionless parameters:

$$Re_q = \frac{u_0}{b_0 E_0}, \quad R_s = \frac{4\pi a D_i L n_p^0}{u_0},$$

where Re_q is the Reynolds electric number, and the parameter R_s characterizes the rate of sticking of the ions to the droplets.

The Poisson equation (7) in dimensionless variables becomes

$$\frac{\partial^2 \varphi^*}{\partial r^{*2}} + \frac{1}{r^*} \frac{\partial \varphi^*}{\partial r^*} + \frac{\partial^2 \varphi^*}{\partial z^{*2}} = -Q(q^* + R_p e_p^* n_p^*), \quad (17)$$

where $Q = 4\pi q_0 L / \varepsilon E_0$ and $R_p = n_p^0 a k T / e q_0$. The parameter Q characterizes the contribution of the space charge of the ions to the variation in the applied electric field, and R_p is the relative contribution of the droplet charge to the space charge of the medium.

Equation (9), which describes the variation in the charge of a particle moving along the trajectory, in the dimensionless form

$$\frac{de_p^*}{dt^*} = \frac{\varepsilon Q q^* I^*}{Re_q} \quad (18)$$

does not contain new dimensionless parameters.

The expression for the total transport current from the nozzle

$$J = 2\pi \int_0^R [(q + q_p)u + qb_i E_z] r dr$$

is written in dimensionless variables as

$$J^* = \int_0^{R^*} [(q^* + R_p e_p^* n_p^*)u^* + \frac{q^* E_z^*}{Re_q}] r^* dr^*.$$

Here R is the radius of the nozzle outlet section BB_1 (Fig. 1) and $J^* = J / (2q_0 u_0 \pi R^2)$.

We give the dimensionless value of the electric-field strength E_w^* on the surface of a stably corona-forming electrode [5]:

$$E_w^* = 12.2\delta[1 + 0.298(r_0\delta)^{-1/2}],$$

where r_0 is the local curvature radius of the corona-forming electrode (needle) and $\delta = \rho / \rho_{nc}$ (ρ_{nc} is the air density under the standard conditions $p = 0.1$ MPa and $T = 293$ K). We recall that the value E_w^* is used in the iterative procedure to calculate the boundary value of the space charge density of the ions q_w^* .

The above problem of nozzle flow of a two-phase mixture containing a gas ionized by a corona discharge and liquid droplets is solved numerically.

Numerical Algorithm. We assign the initial distribution of the space charge density of the ions and droplets (these values are conveniently assumed to be zero over the entire flow region). The Poisson equation (17) is integrated, and the external electric field is determined in a zero iteration. For a numerical solution of (17), we use a finite-element method on triangular grids. Next, from Eq. (16) we determine q^* in the first iteration. Integration of (16) is performed by a difference method on a rectangular grid with specified concentrations. The particle-charge distribution e_p along a certain selected set of trajectories which cover the entire flow region is found by integrating Eqs. (18) using the Runge-Kutta method. Further from (17) we determine a new distribution of the electric potential and the electric-field strength, calculate the boundary value of the variable q^* using (8), again integrate (16), etc. The process of iteration is finished when a steady distribution q^* is attained over the entire flow region. In this case, as already noted, the field strength on the needle surface should have the specified value of E_w^* . In the algorithm described, the time t^* in Eq. (16) is an iteration parameter.

Results of Calculations of the Transport Current from the Nozzle. The receiver conditions and the applied potential difference φ_w were varied. It was assumed that the gas ions are similar in transfer properties to NO^+ ions and the main component of the carrier medium is molecular nitrogen N_2 . The following initial parameters were used: $E_0 = 10^6$ V/m, $L = 0.015$ m, $p_0 = 0.5$ MPa, $T_0 = 373$ K, $a = 10^{-6}$ m, $u_0 = 332$ m/sec, $n_i^0 = 10^{16}$ m $^{-3}$, $\varepsilon = 1$, $\Omega_{ia}^{11} = 0.9$ nm 2 , $G = 10^{-2}$ kg/sec, $\mu_a = 28$, $\mu_i = 30$ a.m.u., $n_p^0 = 1.33 \cdot 10^{14}$ m $^{-3}$. Here Ω_{ia}^{11} is the cross-section of the elastic scattering ion-neutral molecule, μ_a is the molecular weight of the main component of the carrier gas, and μ_i is the molecular weight of the ion.

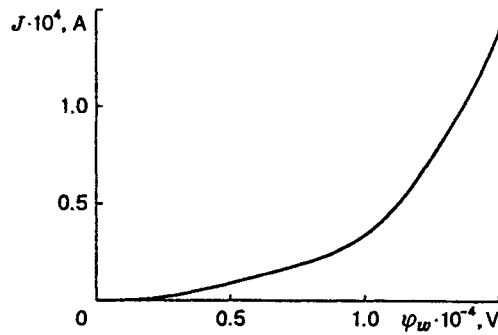


Fig. 2

The nondimensional values computed from the initial parameters have the following values: $Re_q = 2.45$, $R_s = 0.2$, $R_p = 0.297$, and $Q = 2.7$.

Figure 2 shows the transport current J versus the applied potential difference φ_w when the pressure in the receiver is 0.5 MPa. When the pressure in the receiver is $p_0 = 0.2$ MPa and the applied voltage is $\varphi_w = 15$ kV, the transport current is $J = 2.32 \cdot 10^{-4}$ A.

The calculations of the electric current from the supersonic-nozzle outlet with a central corona-forming needle-shaped electrode and the two-phase working medium gas-droplets show that the flow model constructed and the algorithm and programs developed can be used in numerical studies to optimize a device which is a source of charged aerosol.

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