Investigation of motion trajectories of charged microdroplets in electric and gas-dynamic fields

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In this work, mathematical modeling of the motion of charged microdroplets with diameters of 30 and 100 μm under the combined action of electric and gas-dynamic fields is carried out. The structure of the electric field was determined by a system of coaxially located liquid and gas spray capillaries and an annular transport counter electrode. The diameter of the hole in it ranged from 15 to 21 mm; electric potential on capillaries from 2.4 to 5 kV. The pressure excess of the gas at the inlet to the capillary system over the atmosphere ranged from 1 to 6 atm. The numerical integration of the system of Navier-Stokes equations was carried out using the ANSYS Fluent package in an axisymmetric formulation without taking into account the space charge of the droplets.

Keywords: electrospray, transport counter electrode, charged microdroplets, numerical modeling, ANSYS Fluent.

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Introduction

Electrospraying of liquids is the basis of the ionization method used in mass spectrometry of non-volatile molecules Mass-spectrometric experiments revealed that in charged micro- and nanodroplets of the electrospray plume, both simple and complex multistage chemical reactions can take place, sometimes with a significant acceleration compared to their occurrence in the „bulk" [1,2]. The presence of a charge in the droplet is a significant advantage of electrospraying over other methods of generating microdroplets, as it opens up wide possibilities for controlling the parameters of the microdroplet, such as lifetime, size, trajectory. Carrying out chemical reactions in charged micro- and nanodroplets has great potential as the basis of a new method of chemical synthesis — microdroplet chemical synthesis. For problems of microdroplet chemical synthesis, we have proposed a system consisting of coaxially located liquid and gas spray capillaries and a ring transport counter-electrode (TE), between which a spraying potential difference is created. The generated charged micro- and nanodroplets are carried away by the nebulizing gas flow and pass through the TE, and further directed to a suitable sample collector. Such a system is promising for scaling up microdroplet chemical synthesis due to the use of a multiplexed electrospray system. The purpose of this work is to numerically simulate the motion of charged microdroplets in crossed electric and gasdynamic fields without a space charge in the proposed electrospray system to determine its parameters at which the largest number of charged droplets pass through the TE without deposition on it. These include the diameter of the orifice in the TE, the spray voltage and the pressure difference between the pressure at the inlet of the spray capillary and the atmosphere pressure.

1. Simulation Parameters

The geometry used for simulation is shown in Fig. 1. Dimensions are in millimeters. The nebulizing gas is coaxially supplied with the spray capillary from a reservoir behind the boundary. The capillary assembly consists of two capillaries: a round capillary for the liquid fraction supply *3* and an annular capillary for the gas supply *2*. The end of the capillary assembly is in the TE plane. The diameter of the hole in it is selected in the range from 15 to 21 mm in increments of 3 mm. The electric potential on the capillary assembly had values of 5 and 2.4 kV, and on the TE — 0.

The temperature of the gas and the sprayed solution at the inlet to the capillary was 300 K. Methanol with a mass flow rate of $2 \cdot 10^{-9}$ kg/s was taken as a model sprayed liquid. The amount of droplets produced is not directly controlled and is transmitted as a liquid flow rate value. It is assumed that behind the Taylor cone, the droplets disperse in a solid angle of 90 sr, which is given by the starting positions of the particles and the projections of their velocities.

To date, the study of electrospray has focused mainly on mass spectrometry. Therefore, theoretical calculations and simulations are carried out mainly for small charged droplets (up to 10 μm) or their motion near the mass spectrometer interface [4]. Charged droplets from electrospraying are a polydisperse mixture according to their diameters. In the

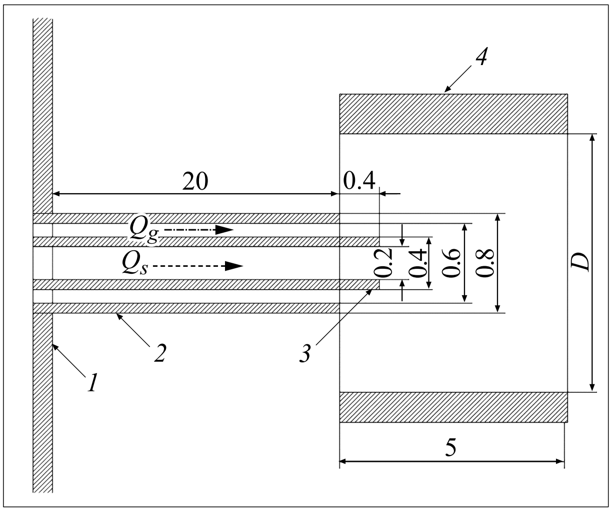

Figure 1. Geometry of the simulated electrospray system: *1* — air reservoir boundary, *2* — gas supply capillary, *3* — solution supply capillary, *4* — TE, *D* — the diameter of the orifice in the TE. The arrows indicate the direction of the sprayed solution with the mass flow rate of the solution Q_s and the gas Q_g.

article of P. Kebarle and W.H. Verkerk [5] it was shown that the range of diameters of droplets formed by electrospraying is from 10 to 100 μm. In the studies [6,7] it has been shown that the average diameter of the droplets is 30 μm. Thus, the initial value of the size of the charged droplets had two values: 30 and 100 μm with charge values of the order of magnitude 10^{-13} and 10^{-12} C, respectively. The charge is defined as 80% of the value obtained from the Rayleigh decay equation [7].

2. Conducting Simulations

Numerical simulation is carried out in three stages: gas-dynamic calculation of the gas flow in the capillary and annular jet, simulation of motion and evaporation of uncharged droplets and then — of charged droplets. The study of the asymptotic behavior of the function on a sequence of meshes with a decrease in the size of the computational cell showed that it is enough to use on the order 140 thousand cells.

In order to find the characteristics of gas flow in a capillary and a ring stream, the system of Navier-Stokes equations in an axisymmetric formulation is used. Numerical integration was performed using the control volume method. To solve the problem, the ANSYS Fluent module version 2021R1 is used. Turbulence is simulated using the k-ω SST turbulence model. The formation of the annular jet is due to the pressure difference at the inlet to the capillary, which is equal to $\Delta p = 6, 4, 2, 1$ atm and the atmosphere. For simulation of motion and evaporation of uncharged droplets, a trajectory problem is solved, i.e. the description of a two-phase medium is performed in a Lagrangian formulation. For determination of the electric field strength in the capillary-ring configuration, the Laplace problem for the potential is solved. The electric field strength vector components are derived using UDF for the ANSYS Fluent software package. The total number of simulated droplets in the quasi-stationary state — when the number of incoming droplets from the source is in equilibrium with the number of droplets leaving the computational domain or depositing on the surface of the ring electrode, — is in the range from $8 \cdot 10^3$ to $4 \cdot 10^4$.

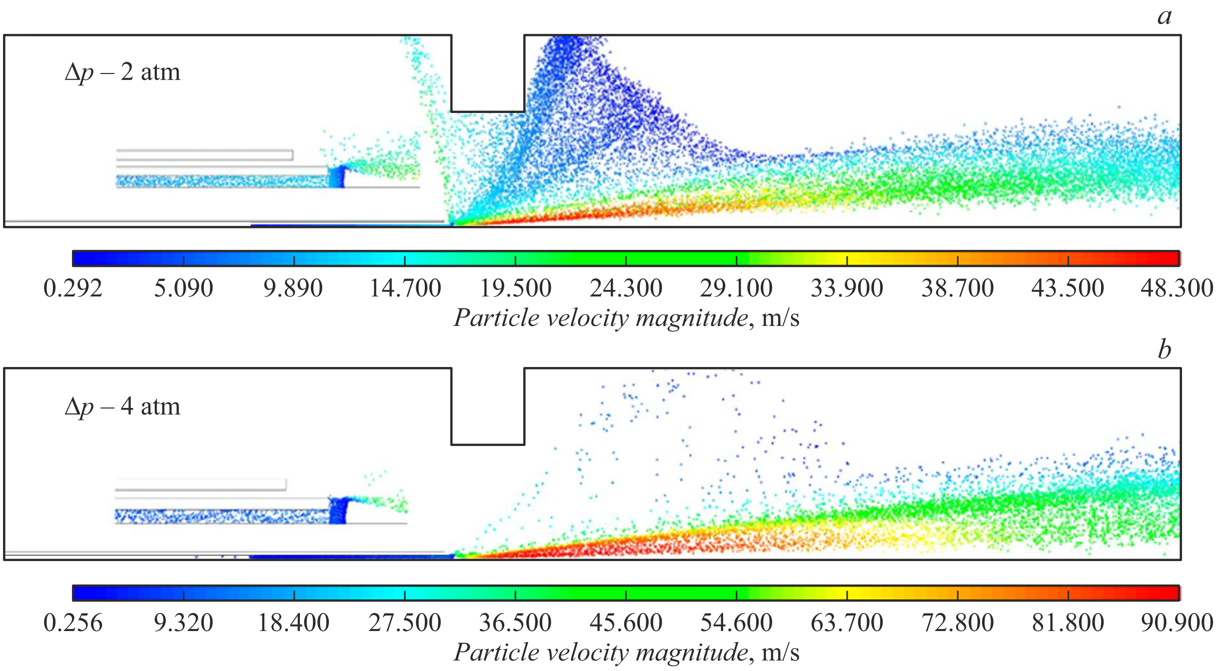

Figure 2. Distribution of Charged Droplets at Different Initial Δp. The hole diameter in the TE is 15 mm, the diameter of the droplets — is 30 μm, the electric potential of the capillary assembly is — 5 kV.

3. Calculation results

For charged microdroplets with a diameter of $30\,\mu$m in the case of $\Delta p = 1-2$ atm, the effect of Coulomb forces is predominant and leads to both a significant change in the trajectories of motion and the deposition of a fraction of particles on the TE. For the rest values of pressure difference and droplets with a diameter of $100\,\mu$m, the influence of Stokes forces is sufficient for the gas flow to carry most of the droplets with it. The results obtained are typical for all the considered values of the potential difference, and when it decreases, the proportion of particles moving towards the TE also decreases. As an example, Fig. 2 shows the two obtained distributions of charged droplets in the TE region and in the space behind it: $\Delta p = 2$ (Fig. $2, a$) and 4 atm (Fig. $2, b$).

In addition, calculations show that droplets with a diameter of $100\,\mu$m have a sufficient initial impulse to remain inaccessible from the electric field and to be only to varying degrees, depending on the pressure difference, subject to Stokes forces, flying away at a smaller angle the greater the value Δp.

Conclusion

Thus, in the numerical simulation of the motion of charged microdroplets in gas-dynamic and electric fields, without considering the space charge, the parameters of the electrospray system at which they pass through the TE region were obtained. This is achieved for microdroplets with a diameter of 30 to $100\,\mu$m, voltages up to 5 kV and $\Delta p = 4$ and 6 atm. Further studies involve experimental verification of the presented results, which will allow expanding the model and considering the volumetric charge.

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Conflict of interest

The authors declare that they have no conflict of interest.

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