Traveling Wave Electrophoresis – Construction of Numerical Model

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Abstract. Numerical model of traveling wave electrophoresis is constructed for a simplified system comprising one continuous electrode and complex system comprising an array of discrete electrodes. It appears that different attractors can coexist in the simplified system – one equilibrium point corresponding to motion with the velocity of the propagating wave and a limit cycle corresponding to slow oscillatory transportation of the charged particle. Coexistence of different attractors builds ground for motion control strategies which can increase the effectiveness of electrophoresis.

Keywords: coexisting attractors, traveling wave, electrophoresis.
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INTRODUCTION

Conveyance of particles and bodies by propagating waves is an important scientific and engineering problem with numerous applications. Manipulation of biological particles and gene expression profiling using traveling wave electrophoresis, particle segregation in suspensions subject to ac electric fields, transport of sand particles and oil spills in coastal waters, transportation of thin films in biomedical applications are just few examples of problems involving interaction between propagating waves and the conveyed objects [1, 2]. A basic model of a particle conveyed by a propagating wave comprises a charged particle in a bed with an array of electrodes mounted at the bottom wall [3]. This produces an electric field wave which travels along the electrodes and interacts with a charged or polarized particle.

Numerical simulation of such a complex nonlinear dynamical problem requires solution of a whole set of problems. Initially, instantaneous electric fields must be reconstructed at different phases of the traveling wave in the analyzed domain. Next, the forces acting to the charged must be approximated in every element of the mesh. Finally, numerical time marching techniques for integration of the governing differential equations describing the motion of the particle must be constructed. This paper presents an overview of the up-mentioned problems and discusses the nonlinear dynamical effects occurring whenever a charged particle interacts with an propagating electric field wave.

A SIMPLIFIED NUMERICAL MODEL

A positively charged particle is located in a two-dimensional viscous bed defined as a half-plane $D:\{-\infty < x < \infty;\ 0 < y < \infty\}$. A continuous electrode is located at the bottom of the bed along the x-axis. It is assumed that a propagating wave of electrical field can be generated on the surface of the continuous electrode:

$$E_0(x) = E\cos(kx - \omega t), \tag{1}$$

where $E_0(x)$ is the electrical field on the surface of the electrode; E is the amplitude of the electrical field wave (on the surface the electrode); k is the wavelength; ω is the circular frequency and t is time. The charged particle interacts with the electrical field and thus forces acting to the particle are generated. It is assumed that these forces are directly proportional to the magnitude of the electrical field at the geometrical location of the particle.

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Quasi-static field of forces acting to the charged particle at $t = 0$ is reconstructed by finite element techniques [X] and is presented in Fig. 1; only one period along the x-axis is shown.

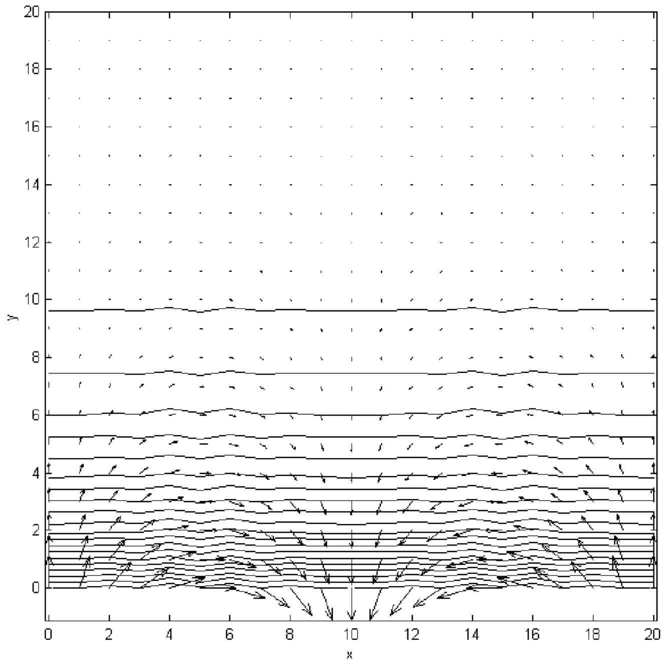

FIGURE 1. Computationally reconstructed field of the quasistatic forces acting to the charged particle; solid lines represent isolines of the magnitude of the force vectors shown at the nodes of the finite element mesh; $E = 0.1$; $k = \pi/10$; $\omega = 1$.

The fact that the izolines of the forces are almost parallel lines enables straightforward approximation of the field of the forces:

$$F_x(x, y, t) = F\exp(-ry)\sin(kx - \omega t);$$
$$F_y(x,y,t) = \begin{cases} F\exp(-ry)\cos(kx - \omega t) \text{ if } y > 0; \\ F\cos(kx - \omega t) \text{ if } ((y = 0) \text{ and } (F\cos(kx - \omega t) \geq 0)); \\ 0 \text{ otherwise.} \end{cases} \quad (2)$$

where F_x and F_y are projections of the forces to the x- and y- axes respectively; F is the magnitude of the force at the surface of the electrode; r is a positive constant defining the decay rate of the force with the increasing distance to the electrode. The composite structure of F_y is determined by the fact that the particle cannot penetrate the electrode.

The value of parameter F can be easily reconstructed from the computational results in Fig. 1 (the magnitude of the force vector lengths at the same elevation from the surface of the electrode is almost the same): $F = 1.1130$. Reconstruction of parameter r requires application of computational minimization algorithm based on least squares. We minimize the residual constructed as the sum of squared differences between the approximated and computationally reconstructed fields of forces:

$$\min_r \left(\sum_{j=1}^{21} \left(3.1130\exp(-r(j-1)\delta_y) - \frac{1}{21}\sum_{i=1}^{21} \sqrt{\hat{F}_x^2((i-1)\delta_x, (j-1)\delta_y, 0) + \hat{F}_y^2((i-1)\delta_x, (j-1)\delta_y, 0)} \right)^2 \right), \quad (3)$$

where δ_x and δ_y are steps of the finite element mesh in the direction of x- and y- axes. The resulting value of parameter r is $r = 0.312$. Now, the approximated field of forces can be used to construct the governing equations of motion of a charged particle in a viscous bed with a continuous electrode generating a propagating electrical field:

$$\begin{cases} m\ddot{x} + h\dot{x} = F_x(x, y, t); \\ m\ddot{y} + h\dot{y} = F_y(x, y, t), \end{cases} \tag{4}$$

where m is the mass of the particle; h is coefficient of the linear viscous damping force; top dots stand for full derivatives by time.

EQUILIBRIUM POINTS AND COEXISTING ATTRACTORS

The dynamical system described by eq. (4) and eq. (2) has an equilibrium point at:

$$\left\{ \ddot{x}_0 = 0; \quad \ddot{y}_0 = 0; \quad \dot{x}_0 = \frac{\omega}{k}; \quad \dot{y}_0 = 0; \quad x_0 = \frac{\omega}{k} t + \theta; \quad y_0 = 0 \right\}, \tag{5}$$

where θ is a phase shift between the geometrical location of the particle sliding on the surface of the electrode and the nearest peak of the propagating wave. The conditions of the existence of the equilibrium point yield:

$$h\frac{\omega}{k} = F\sin(k\theta); \; F\cos(k\theta) \le 0. \tag{6}$$

The second condition of existence in eq.6 is necessary to keep the particle on the surface of the electrode – otherwise the particle would be pushed away from the surface of the electrode. There exist two sets of phases of the equilibrium point:

$$\theta_1 = \frac{1}{k}\left(\arcsin\left(\frac{h\omega}{kF}\right) + 2\pi n \right); \; \theta_2 = -\frac{1}{k}\left(\arcsin\left(\frac{h\omega}{kF}\right) + (2\pi + 1)n \right); \; n \in Z. \tag{7}$$

It is clear that the first type equilibrium points do not satisfy the conditions of existence (eq.6). Equilibrium point describes a particle sliding on the surface of the electrode. Thus the stability of the equilibrium points can be determined from the simplified equation $m\ddot{x} + h\dot{x} = F_x(x, 0, t)$. Thus, the eigenvalues of the Jakobi matrix of the linearised system in the surrounding of the equilibrium point are:

$$\lambda_{1,2} = \frac{-h \pm \sqrt{h^2 + 4mF\cos(k\theta)}}{2m}, \tag{8}$$

As noted previously, equilibrium points of the first type do not satisfy the necessary conditions of existence. Nevertheless, we will calculate eigenvalues for both types of equilibrium points. The eigenvalues of the first type equilibrium point are real numbers, one positive, another – negative (because $\cos(k\theta_1) > 0$). Thus, it is a saddle point. The second type equilibrium point is a stable equilibrium point (focus or knot depending from the magnitude of F).

Saddle points are very important equilibrium points in nonlinear dynamics [4]. Integration backwards in time from the surroundings of the saddle point may help to construct basin boundaries of the coexisting attractors. In [5] unstable saddle points are exploited for construction of a control strategy of transient solutions. In our system the saddle point does not exist. It is impossible to find such a direction of motion towards the first type equilibrium point (a separatrix) that an approaching particle in that direction would stay for an infinitely (theoretically) long time in the surroundings of that point. The field of forces would push the particle away from the electrode – the force component F_y is always positive in the surrounding of the first type equilibrium point.

But the second type equilibrium point does exist. It corresponds to a continuous motion of the particle on the surface of the electrode with a constant velocity equal to the velocity of the propagating charge wave. Clearly, the stable equilibrium point is not the only motion mode of the particle in two-dimensional area D. Numerical simulation techniques are developed to investigate the dynamics of the particle not only sliding on the electrode, but also moving in the viscous media above the electrode. It appears that there exist two different regimes of motion which are sensitive to the initial conditions: motion with the velocity of the propagating wave (on the surface of the electrode) and cyclic motion with slow average velocity above the electrode.

The fact that different types of motion coexist builds the ground for effective motion control strategy. Initial variation of the speed of the propagating wave, initial displacement or velocity of the particle can change the processes of transient dynamics from relatively slow cyclic transportation to efficient motion with the speed of the propagating wave.

NUMERICAL MODEL COMPRISING DISCRETE ELECTRODES

Analogous numerical model is built for a similar problem with the exception that the electrode placed at the bottom of the bed is discrete. Every separate electrode generates its electrical field and the quasistatic field of forces acting to the charged particle is calculated as the superposition of fields generated by eight electrodes. Again, the propagating wave of electrical potential is constructed and though the governing equations of motion are analogous to the ones in eq.(4), the terms F_x and F_y are recalculated at every time step. The distribution of the field of forces at $t = 0$ is presented in Fig. 2.

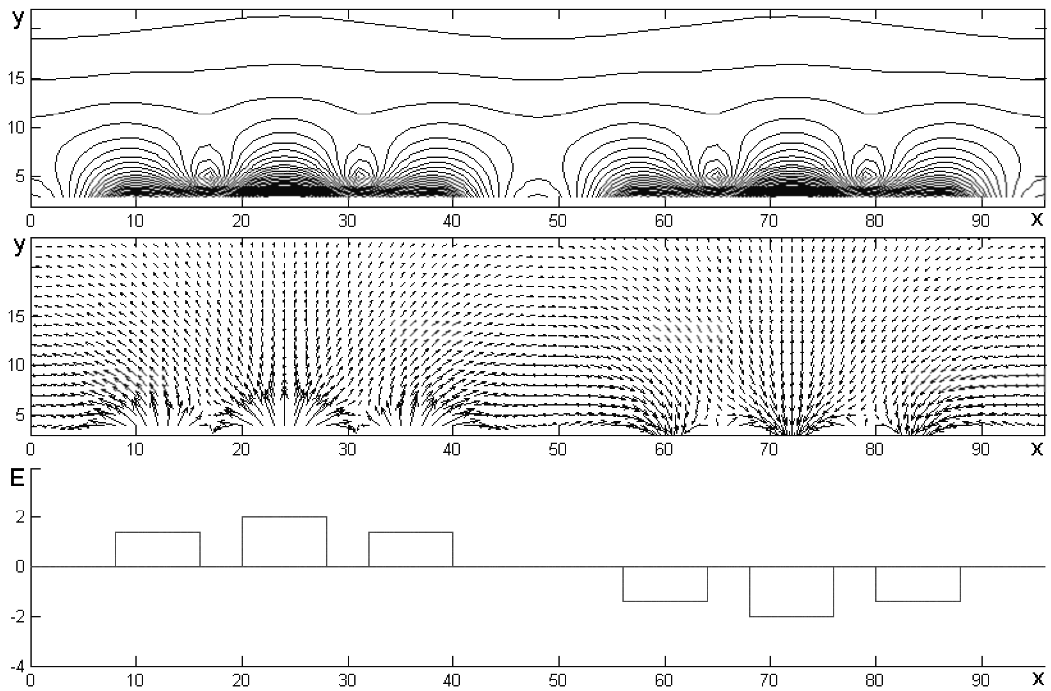

FIGURE 2. Computationally reconstructed field of the quasistatic forces acting to the charged particle generated by eight electrodes; solid lines represent isolines of the magnitude of the force vectors shown at the nodes of the finite element mesh; block diagrams represent electric fields at appropriate electrodes; $E = 0.1$; $k = \pi/50$; $\omega = 1$.

Numerical simulations of the process of electrophoresis by such an array of discrete electrodes also confirm the fact that two different regimes of motion can coexist at certain sets of parameters. The fact can be exploited for development of effective motion control strategies what is a definite object of future research.

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