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Hydrodynamics, Gravitational Sensitivity, and Transport Phenomena in Continuous Flow Electrophoresis

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Abstract

A MULTIZONE mathematical model for hydrodynamics, heat and mass transfer in continuous flow electrophoresis (CFE) is reported. The model divides the electrophoretic cell into three zones: the entrance region, the zone of the mixture injection, and the zone of the parallel fluid flow. Three-dimensional transport equations, including Navier-Stokes equations, and equations of heat and mass balance are significantly simplified in each zone. The length of the cell entrance region and recirculation flows in the CFE cell are found to be affected by thermal convection caused by internal heating of the fluid. The influences of convective diffusion and electro-osmosis on concentration profiles of separated fractions are studied numerically for a wide range of the Peclet number.

Contents

A possibility to scale up a cell of a CFE instrument by eliminating thermal convection in microgravity predestined a series of experiments with CFE in space.[1] The cell is a gap between two parallel thermostatic plates through which an electrolyte water solution and a mixture to be separated are pumped. The width of the cell is much less than its length and height to suppress thermal convection caused by internal Joule heating. The throughput and resolution of the CFE depend on the character of the fluid flow. The flow should be laminar, steady, and with parallel streamlines (parallel flow). In practice, there are distortions of the parallel flow due to forced and thermal convection. This paper presents a mathematical model that is able to study the structure of the fluid flow in the CFE cell as well as the influence of the Peclet number and electro-osmosis on concentration profiles.

The mathematical model for fluid flow and transport processes assumes that concentrations of the mixture components and ions in the solution are much less than the concentration of the solvent (water) and do not affect the fluid flow, electroneutrality approximation is valid, diffusion currents of ions are negligible, fluid is incompressible and Newtonian, chemical reactions do not occur during electrophoretic separation, the Boussinesq approximation is valid, diffusion boundary layers appearing near the electrodes are negligibly thin, and electrohydrodynamical effects are neglected.

These assumptions lead to a three-dimensional set of equations governing viscous fluid flow and heat/mass transfer in the CFE cell. Since the cell width is much less than its length and height, the space of the cell is divided into three zones and the governing equations are simplified according to the peculiarities of these zones. The following zones are distinguished in the cell domain: the entrance region where the parallel flow forms, the zone of the mixture injection, and the zone of the parallel flow where the electrophoretic separation occurs. The entrance region length determines the position where the mixture is injected into the fluid flow and, hence, the upper bound of the second zone. A boundary condition for the third zone is found as a result of fluid flow and mass transfer modeling in the second zone.

In the first zone, velocity components lying in the plane of the cell and the temperature of the fluid are represented by polynomials of the second power of the coordinate x corresponding to the shortest side of the cell, and Navier-Stokes equations are averaged over this coordinate[2,3]:

$$\frac{6}{5}\left(v_y\frac{\partial\omega}{\partial y}+v_z\frac{\partial\omega}{\partial z}\right)=\frac{G}{3Re^2}\frac{\partial\vartheta}{\partial z}+\frac{1}{Re}\left[\frac{\partial^2\omega}{\partial y^2}+\frac{\partial^2\omega}{\partial z^2}-3(l/d)^2\omega\right] \tag{1}$$

$$\omega=\frac{\partial^2\psi}{\partial y^2}+\frac{\partial^2\psi}{\partial z^2} \tag{2}$$

$$\frac{6}{5}\left(v_y\frac{\partial\vartheta}{\partial y}+v_z\frac{\partial\vartheta}{\partial z}\right)=\frac{1}{RePr}\left[\frac{\partial^2\vartheta}{\partial y^2}+\frac{\partial^2\vartheta}{\partial z^2}-3(l/d)^2\vartheta\right] \tag{3}$$

$$v_y=-\frac{\partial\psi}{\partial z},\quad v_z=\frac{\partial\psi}{\partial y},\quad T_c=\frac{qd^2}{\chi},\quad \delta T_0=T_0-T_w$$

$$G=\frac{g\beta(3\delta T_0-T_c)l^3}{\nu^2},\quad Re=\frac{\langle V\rangle l}{\nu},\quad Pr=\frac{\rho C_p\nu}{\chi}$$

where y and z are the dimensionless coordinates; ψ, ω, and ϑ are the averaged dimensionless stream function, vorticity, and temperature; l is the half-length of the cell used as a space scale; d is the half-width of the cell; v_y and v_z are the fluid velocity components; G, Re, and Pr are the Grashof, Reynolds, and Prandtl numbers; C_p, ρ, β, ν, and χ are the specific heat capacity, density, coefficient of thermal expansion, kinematic viscosity, and thermal conductivity of the fluid; T_c is the characteristic temperature; T_0 and T_w are the inlet and the wall temperatures; g is the acceleration due to gravity; q is the heat generation rate; and $\langle V\rangle$ is the average cross-sectional velocity.

Boundary conditions for Eqs. (1-3) are no-slip conditions for Eqs. (1) and (2) and adiabatic conditions for Eq. (3) at the rigid boundaries; the axial velocity and the temperature at the inlet are taken equal to l/s and 1, respectively, where s is half of the inlet size. At the outlet, the axial temperature derivative is equal to zero, and the axial velocity is equal to unity.

Flow structure and the entrance region length were numerically investigated for various Grashof and Reynolds numbers to elucidate the mechanism of the CFE gravitational sensitivity. It was shown that differences in the average temperature of the entering fluid and the fluid remote from the entrance can generate either a jet for negative values of the Grashof

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number or boundary layers for positive ones. The jet may cause reverse flows mixing the separated fractions.

Numerical experiments for the zero Grashof number showed that CFE operation under zero-gravity conditions does not guarantee improvement of the CFE separation because increase in the cell width leads to formation of reverse flows at the entrance of the cell.

Two-dimensional Navier-Stokes equations are used for the second zone that is the region of the mixture injection. This zone is the confluence of the mixture and the buffer flows. It is assumed that the mass transfer in this zone is mainly determined by convection and diffusion, whereas the electrophoretic displacement is negligible. Our calculations showed that, for the Reynolds numbers characteristic for the CFE and for reasonable injector dimensions and mixture flow rates, reverse flows did not occur. The mixture concentration at the lower boundary of the zone has a stepwise form.

In the zone of electrophoretic separation, the flow and temperature fields become fully developed and depend on the transverse coordinate x only. It is assumed that the fluid viscosity and conductivity depend linearly on its temperature. The general set of equations is reduced to one-dimensional Navier-Stokes equations for fluid flow and a parabolized three-dimensional convection-diffusion equation for the concentration of the mixture component. The mass balance equation for a mixture component is further simplified owing to the very large axial Peclet number. The axial diffusion flux is neglected and a parabolized form of the steady convection-diffusion equation is given by

$$v_y \frac{\partial C}{\partial y} + \left(v_z + \frac{\mu E}{\bar{v}}\right) \frac{h}{d} \frac{\partial C}{\partial z} = \frac{h}{dPe} \left(\frac{\partial}{\partial x} D \frac{\partial C}{\partial x} + D \frac{\partial^2 C}{\partial z^2}\right) \quad (4)$$

where $(\partial C/\partial x) = 0$ at $x = \pm 1$, $C = 0$ at $z = \pm\infty$, $C(x, 0, z) = C_0(x, z)$, and $Pe = \bar{v}d/D^c$ where C is the dimensionless local concentration, D the dimensionless diffusivity, E the intensity of the electric field, Pe the diffusional Peclet number, μ the electrophoretic mobility, D^c the characteristic diffusivity, h the height of the electrophoretic separation zone, and $\bar{v}$ the average axial velocity of one-dimensional flow that differs from the average cross-sectional average velocity $\langle V \rangle$ by the value proportional to d/l. The axial coordinate y is measured in units of h, x and z are measured in the units of the cell half-width d, and $C_0(x, z)$ is the concentration at the upper bound of the zone found as a result of the modeling for the second zone.

Parameter $h/(dPe)$ represents a ratio of the residence time of a mixture component in the CFE cell to its characteristic diffusion time and, thus, indicates the effect of diffusion on the concentration distribution at the outlet of the cell. The final stage of the modeling is the calculation of a concentration profile F that is defined as y mass flux distribution over z coordinate at the outlet plane of the chamber and is given by

$$F(z) = \int_{-1}^{+1} v_y C|_{y=1} \, dx \quad (5)$$

The limiting cases of large and small Pe have been analyzed in previous studies.[4-6] We applied our model to find the behavior of the concentration profile in the whole range of the parameter $h/(dPe)$. Concentration profiles calculated for different values of $h/(dPe)$ are shown in Fig. 1. It is seen from the figure that in the case of small values of $h/(dPe)$ diffusion leads to an increase of the tail of the concentration profile (curves 1 and 2). Curve 3 shows that for $h/(dPe) = 0.7$ dispersion increases and the maximum of the concentration profile shifts in the direction of the electrophoretic motion. Further increase in $h/(dPe)$ causes a decrease of dispersion (curve 4) and then leads to its growth (curve 5).

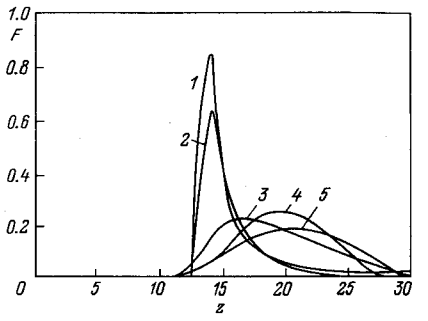

Fig. 1 Influence of diffusional parameter $h/(dPe)$ on the position and dispersion of concentration profiles: $h/d = 200$, $\mu E/\bar{v} = 0.1$, 1) $h/(dPe) = 0.01$, 2) $h/(dPe) = 0.1$, 3) $h/(dPe) = 0.7$, 4) $h/(dPe) = 3.5$, 5) $h/(dPe) = 8$.

Results of the modeling show that the dependence of the dispersion of the concentration profile on the parameter $h/(dPe)$ is not monotonous and the position of the concentration profile depends on $h/(dPe)$. These effects should be taken into account when planning space experiments and comparing data obtained in space on a wide-gap cell with that obtained in terrestrial experiments by using a narrow-gap cell.

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