COMPUTER SIMULATION OF FREE FLOW ELECTROPHORETIC SEPARATION

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ABSTRACT: A mathematical model for three-dimensional laminar steady flow of an incompressible viscous neutrally charged carrier fluid injected with a fluid mixture having differently electrically charged particles was presented. All magnetic fields have been neglected. Thermally induced buoyancy was incorporated via an extended Boussinesq approximation while including Joule heating effect. Numerical results demonstrate detrimental effects of numerical dissipation on the accuracy of the solution. Bending and separation of the injected stream of differently charged particles under the influence of an electric field and formation of electroconvective and thermoconvective vortices were successfully demonstrated.

I. INTRODUCTION

Electrohydrodynamics (EHD) and Magnetohydrodynamics (MHD) are representing two extreme models for a general fluid flow under the influence of electromagnetic fields [1]. The EHD model assumes that there is no magnetic field applied or induced [2], while MHD model assumes that there are no charged particles in the flow field and that there is no electric potential applied [3]. In EHD flows external electric field is applied to a fluid containing electricaly charged particles [4-6]. Applications of EHD flows range from ink-jet printers to electrophoretic separation processes [7-15]. Only incomplete models of EHD flows have been numerically solved in the past.

II. MODELLING

Mathematical model presented in this paper consists of a neutral carrier fluid with several species of charged particles. This model can be easily extended to non-neutral carrier fluids.The system of governing equations is derived from a combination of Maxwell's equations of electrodynamics and the Navier-Stokes equations. Idealized charged fluid is assumed and therefore magnetic fields can be neglected. Maxwell's equations reduce to a charge conservation equation for each of the charged species and equation for electric potential. For computational purposes system of equations can be written in fully conservative vector form in general ξ,η,ζ curvilinear non-orthogonal coordinates as follows:

$$\frac{\partial \tilde{Q}}{\partial t}+\frac{\partial \tilde{E}}{\partial \xi}+\frac{\partial \tilde{F}}{\partial \eta}+\frac{\partial \tilde{G}}{\partial \zeta}=\frac{\partial}{\partial \xi}\left(\frac{\tilde{D}}{J}\, g_{ij}\, \frac{\partial J\tilde{Q}}{\partial \xi}\right)+\frac{\partial}{\partial \eta}\left(\frac{\tilde{D}}{J}\, g_{ij}\, \frac{\partial J\tilde{Q}}{\partial \eta}\right)+\frac{\partial}{\partial \zeta}\left(\frac{\tilde{D}}{J}\, g_{ij}\, \frac{\partial J\tilde{Q}}{\partial \zeta}\right)+\tilde{S} \quad (1)$$

To make system of equations (1) non-singular and hyperbolic in time, artificial compressibility concept was applied [16] and p/β term was added to the mass conservation equation. Solution vector, flux and source term vectors in curvilinear coordinates and non-dimensional form are:

$$\tilde{\mathbf{Q}} = \frac{1}{J}\begin{Bmatrix} p/\beta \\ u \\ v \\ w \\ \theta \\ q \end{Bmatrix} \quad \tilde{\mathbf{E}} = \frac{1}{J}\begin{Bmatrix} U \\ Uu+\xi_x p \\ Uv+\xi_y p \\ Uw+\xi_z p \\ U\theta \\ q(U+\frac{1}{\mathrm{RePr_E}}E_\xi) \end{Bmatrix} \quad \tilde{\mathbf{F}} = \frac{1}{J}\begin{Bmatrix} V \\ Vu+\eta_x p \\ Vv+\eta_y p \\ Vw+\eta_z p \\ V\theta \\ q(V+\frac{1}{\mathrm{RePr_E}}E_\eta) \end{Bmatrix} \tag{2}$$

$$\tilde{\mathbf{G}} = \frac{1}{J}\begin{Bmatrix} W \\ Wu+\zeta_x p \\ Wv+\zeta_y p \\ Ww+\zeta_z p \\ W\theta \\ q(W+\frac{1}{\mathrm{RePr_E}}E_\zeta) \end{Bmatrix} \quad \tilde{\mathbf{S}} = \frac{1}{J}\begin{Bmatrix} 0 \\ \frac{Gr}{Re} n_x + S_E q E_x \\ \frac{Gr}{Re} n_y + S_E q E_y \\ \frac{Gr}{Re} n_z + S_E q E_z \\ S_E\, Ec\left[q\left(v+\frac{1}{\mathrm{RePr_E}}E\right) - \frac{1}{\mathrm{ReD_E}}\nabla q\right]\cdot E \\ 0 \end{Bmatrix} \tag{3}$$

Electric charges are related to electric potential field, that is,

$$\nabla^2 \Phi = -N_E q \tag{4}$$

where the electric field is $E = (E_x, E_y, E_z)$. The Jacobian determinant of the geometric transformation from physical into computational space is $J = \frac{\partial(\xi,\eta,\zeta)}{\partial(x,y,z)}$, g_{ij} is the contravariant metric tensor, $v=(u,v,w)^T$ denotes velocity field with U,V,W as its contravariant components, p is the pressure, q are the electric charges concentration, θ is the nondimensional temperature, and Φ is the electric potential, while $\tilde{\mathbf{D}} = (1/Re)\,\mathrm{diag}(0, 1, 1, 1/Pr, 1/D_E)$. Non-dimensional numbers such as Reynolds number Re, Prandtl number Pr, Eckert number Ec, Grashof number Gr are defined in a standard way while electrical characteristic numbers are defined [3] as:

Charge diffusivity characteristic

Lorentz force characteristic

$$D_E = \frac{\mu_r}{\rho_r D_r} \qquad S_E = \frac{q_r \Phi_r}{\rho_r v_r^2} \tag{5}$$

Electric Prandtl number   Electric field characteristic

$$Pr_E = \frac{\mu_r}{\rho_r b_r \Phi_r} \qquad N_E = \frac{q_r l_r^2}{\varepsilon_r \Phi_r} \tag{6}$$

In the equations above ρ represents density, l characteristic length, μ dynamic viscosity, ε electrical permitivity, while subscript r denotes reference values. Diffusivity coefficient D and mobility coefficient b are related by the Einstein's relation [10]. It should be noted that the electric permitivity ε is assumed to be uniform. System of equations given by (1) is solved using four stage Runga-Kutta explicit time stepping method [17]. Second and fourth order artificial dissipation were judiciously added to minimize numerical oscillations.

III. RESULTS

The test case was a simple model for steady flow in a rectangular electrophoresis chamber of the width l = 0.1 m. A charged fluid was injected at the centerline of the main inlet to the left of the chamber at the same speed as the aqueous electrically neutral carrier fluid. Both fluids were assumed to have the same density. Temperature was constant along the boundaries and Joule's heating and buoyancy force effects were neglected, so that heat transfer effects were not taken into account. A computational grid consisting of 60 × 60 nonclustered cells was used to discretize the flow domain having an aspect ratio AR = 10 with the mean flow running from left to right. Initially, charges were specified along the centerline of the entire length of the chamber. A fully developed parabolic velocity profile for the carrier fluid throughout the flowfield and a linear variation of the electric potential between the top and bottom walls were used as initial conditions. A constant electric potential difference of 20 Volts was applied at every station across the passage starting from the inlet until exit. The nondimensional numbers used in this test case were:

$Re = 100$, $Pr = 7.936$, $Gr = 0$, $Ec = 8.6 \times 10^{-9}$, $N_E = 14.4$, $Pr_E = 1.001$, $S_E = 1.66 \times 10^{-3}$, $D_E = 2.5 \times 10^{7}$. As a consequence of the imposed electric field, the charged fluid was deflected from the centerline (Fig. 1a) as it was carried by the carrier fluid which developed a typical Poiseuille velocity profile (Fig. 1b) along the chamber. Computed lines of equal electric potential (Fig. 1c) and isobars (Fig. 1d) similarly do not indicate any significant perturbation due to the week concentration of the electric charges in the stream and the low level of the imposed electrical field. Since the nondimensional charge density at the inlet boundary was specified as smoothly varying over nine grid points (having a value of one at the centerline), the given case represented a difficult task from a numerical point of view. We have attempted to overcome this problem by explicitly adding a small amount of fourth order artificial dissipation. However, it was found that even a very small amount of artificial dissipation necessary to enhance the convergence rate has a detrimental effect on the accurate prediction of the diffusion of charged particles. By trial and error, it was found the combined artificial dissipation of second and fourth order with coefficients having values of $\varepsilon_2 = 0.005$ and $\varepsilon_4 = 0.0004$ gave acceptable results. Specifically, for the case when the electric potential difference was $\Delta\varphi = 20$ Volts, the predicted electric charge density profiles at different stations along the channel (Fig. 2) indicate slight bending and diffusion of the charged particle stream, while accurately preserving global charge conservation at every station. Figure 3 depicts the monotonic convergence history of the iterative process where the grid point normalized sum of the residuals of the system is plotted versus the number of iterations. All computations were performed on Cray-YMP computer at NASA Ames Research Center.

IV. REFERENCES

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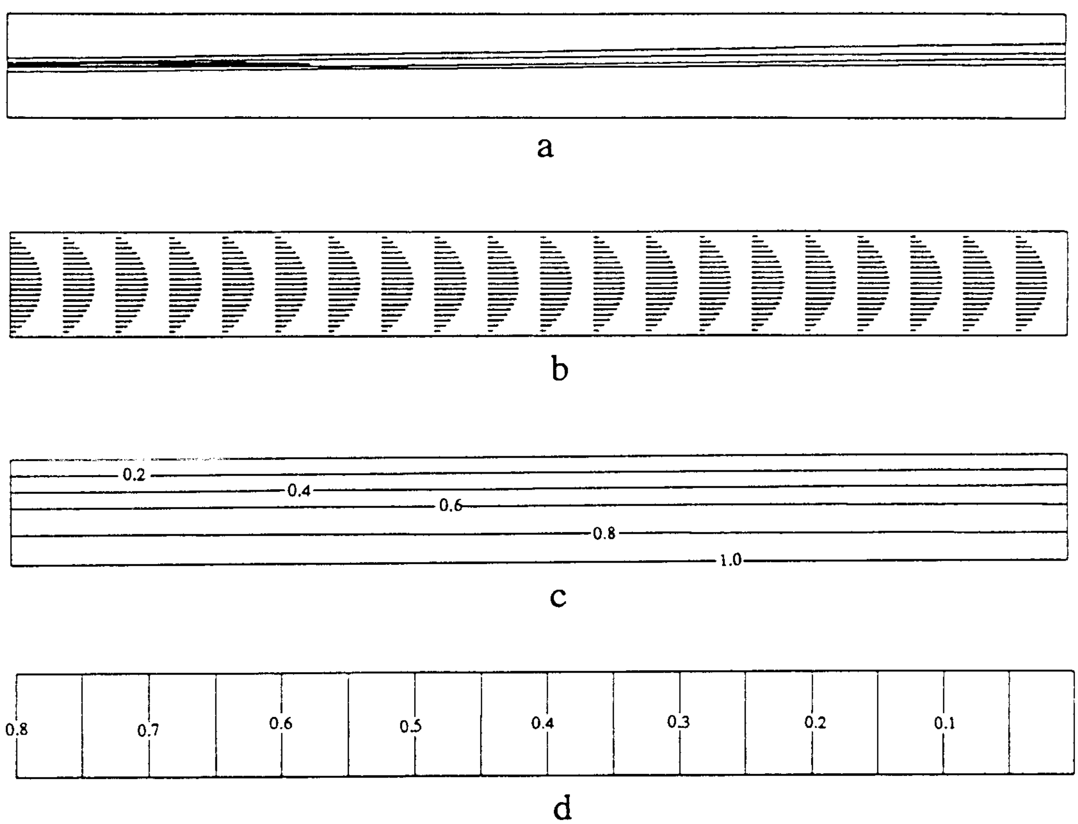

Figure 1. Free flow electrophoretic separation simulation: a) constant electric charge density lines, b) velocity vector profiles, c) electric field iso-potential lines, and d) isobars.

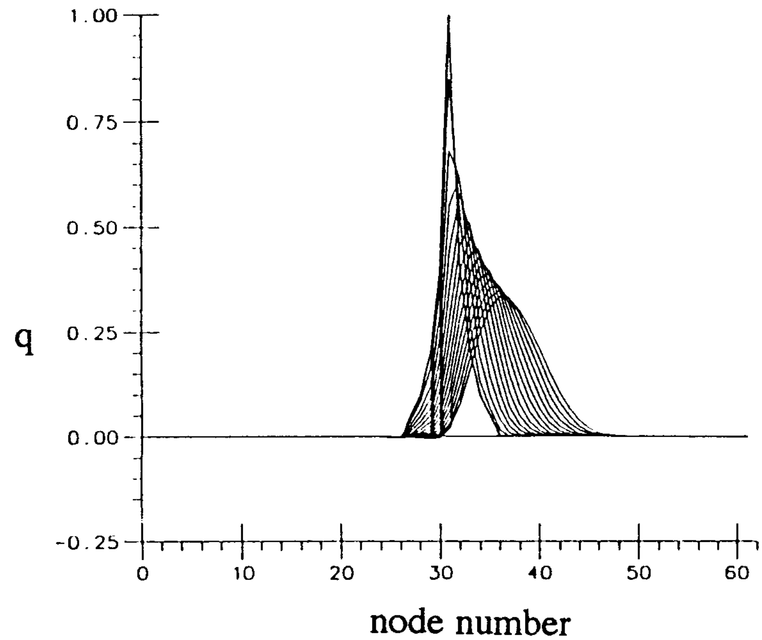

Figure 2. Electric charge density profiles at different stations along the channel

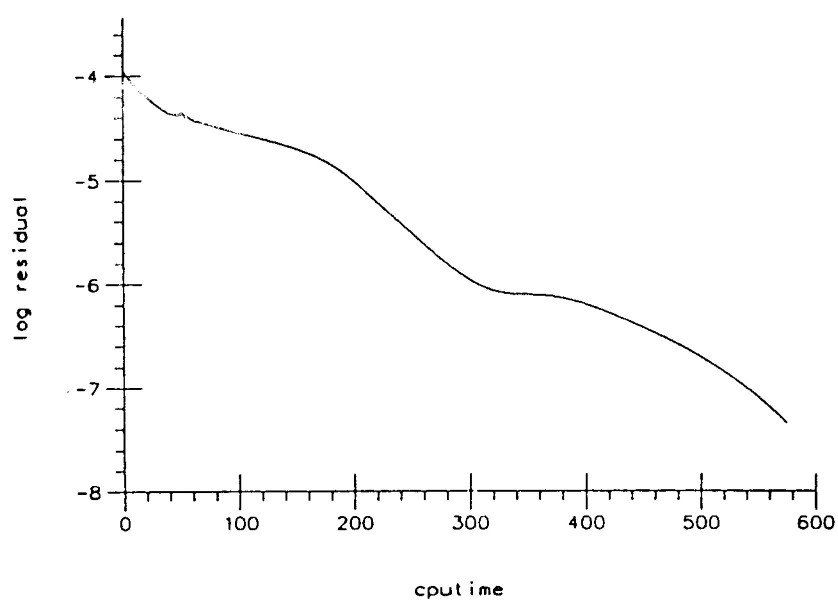

Figure 3. Convergence history of the iterative process