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Viscoelastic Effects on Dispersion due to Electroosmotic Flow with Variable Zeta Potential

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Abstract **-** In this work the influence of viscoelasticity and wall zeta potential effects on the dispersion coefficient of an electroosmotic flow through a micro-channel is studied. The governing equations for the fluid are reduced in the limit of the lubrication approximation theory (LAT). For the symmetric electrolyte, the Poisson-Boltzmann equation was solved by considering the wall zeta potential changes axially by the relationship $\zeta(x) = \zeta_0 + \Delta\zeta \sin\frac{2\pi x}{L}$. Here ζ_0 is a reference wall zeta-potential, $\Delta\zeta$ is the amplitude of the fluctuations of the periodic function $\zeta(x)$, x and L are the axial variable and the micro-channel length, respectively. The simplified equations are solved numerically to determine the axial distribution of the dispersion coefficient as a function of the main parameters involved in the analysis.

Keywords**:** Electroosmotic flow; Viscoelastic; Taylor Dispersion; Variable Zeta-Potential

1. Introduction

To improve the mixing process in microfluidics devices, recently electrokinetics pertaining to non-Newtonian fluids have been studied. The coupling between non-Newtonian hydrodynamics and electrostatics not only complicates the electrokinetics but also causes a distorted velocity profile through the micro-channel that can contribute directly to the dispersion process. In this sense, C. Zhao et al. [1] analyzed an electroosmotic flow of power-law fluids in a slit channel with constant wall potential. They demonstrated that the velocity profile becomes less plug-like as the fluid behavior index increases, n. Also, they found that for pseudoplastic liquids, $n < 1$, the generalized Smoluchowski velocity can be several times that of the conventional Smoluchowski velocity, and thus the electrokinetic flow rate can be significantly higher than that for Newtonian fluids. Similar results with high zeta potentials in the walls of the micro-channel are found in [2]. The analysis of the electrokinetic flow of a power-law fluid through a slit channel with gradually varying wall potential and channel height was reported in [3,4]. They found that the interaction between the wall undulation and the wall potential modulation, under the combined action of hydrodynamic and electric forces, may give rise to a rich set of nonlinear behaviors for flow of a non-Newtonian fluid in the channel. Recently O. Bautista et al. [5], studied the problem of the purely electro-osmotic flow of a viscoelastic liquid, which obeys the simplified Phan-Thien-Tanner (sPTT) constitutive equation, is solved numerically and asymptotically by using the lubrication approximation. The authors included Joule heating effects caused by an imposed electric field, where the viscosity function, relaxation time and electrical conductivity of the liquid are assumed to be temperature- dependent considering the zeta-wall potential constant. Hence in the present work, we study the hydrodynamic dispersion due to an electro-osmotic flow of a viscoelastic fluid for high Deborah numbers, in a micro-channel considering that the wall zeta potential varies in axial direction according to a sinusoidal function [6].

2. Mathematical Formulation

In Figure 1 we present a qualitative sketch for the steady hydrodynamic dispersion in a purely electroosmotic flow through a micro-channel formed by two parallel plates, where the length (L) of the micro-channel is much greater than the plate separation ($2H$). The transverse coordinate is y to be vertical and x is the horizontal coordinate. At $y = \pm H$, let the upper and lower walls be sinusoidally modulated with a slowly axially varying zeta potential $\zeta(x)$.

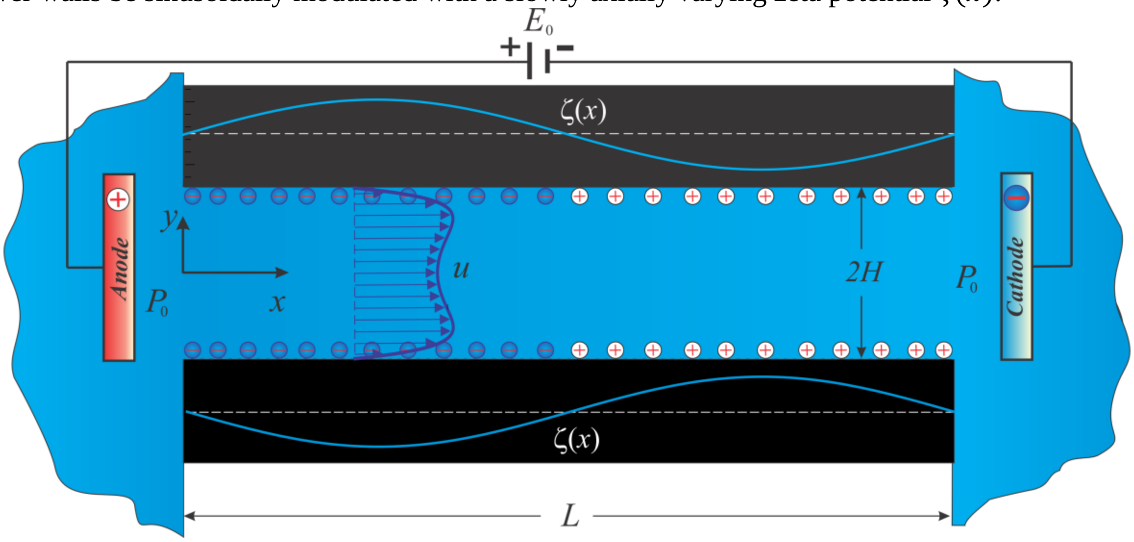

Fig. 1: Physical model under study.

The fitting dimensionless variables and parameters used in the present work are defined by the following relationships reported by O. Bautista et al. [5],

$$\chi = \frac{x}{L}, Y = \frac{y}{H}, \tilde{u} = \frac{u}{U_{HS}}, \tilde{v} = \frac{vL}{U_{HS}H}, \tilde{P} = \frac{(p' - P_0)H^2}{\eta_0 U_{HS} L},$$
$$\tilde{\tau}_{xy} = \frac{\tau_{xy} H}{\eta_0 U_{HS}}, \tilde{Q} = \frac{Q}{2U_{HS}H}, \tilde{\psi} = \frac{\psi}{\zeta_0}, \tilde{\zeta} = \frac{\zeta(x)}{\zeta_0}, \tag{1}$$
$$\tilde{\kappa} = \kappa H, \beta = \frac{H}{L}.$$

In the above, (χ, Y) are the axial and transversal dimensionless coordinates, U_{HS} is the Helmholtz-Smoluchowski velocity [7], (u, v) represent the axial and transversal components of the velocity in physical units, $(\tilde{u}, \tilde{v})$ correspond to the dimensionless axial and transversal components of the velocity, $(P_0, \tilde{P})$ are the pressure in physical units at entrance and exit of the micro-channel and in dimensionless form, respectively. η_0 is the viscosity, $(Q, \tilde{Q})$ are the volumetric flow rate in physical units and in dimensionless form, respectively. Also $(\tau_{xy}, \tilde{\tau}_{xy})$ represent the shear stresses in physical units and in dimensionless form. The electric potential into the electrical double layer (EDL) in physical and dimensionless form are $(\psi, \tilde{\psi})$, then the solution of the Poisson-Boltzmann equation is $\tilde{\psi} = \tilde{\zeta} \cosh \tilde{\kappa} Y / \cosh \tilde{\kappa}$, here $\tilde{\zeta}$ represents the dimensionless variable zeta potential. $(\kappa, \tilde{\kappa})$ are the inverse of the Debye length in physical units and in dimensionless form [7]. The parameter β is a geometric relationship parameter and we assume that it is small in comparison with the unity. It was useful to define $p' = p - \tilde{\varepsilon}\, \kappa^2 \psi^2 / 2$ used in [8], where $\tilde{\varepsilon}$ represents the dielectric permittivity of the fluid. On the other hand, in the limit of the LAT, $\beta \ll 1$ and after using the aforementioned dimensionless variables, the momentum equation and the constitutive equation for the modified PTT model is reduced as [5],

$$-\frac{d\tilde{P}}{d\chi} + \frac{\partial \tilde{\tau}_{xy}}{\partial Y} + \tilde{\kappa}^2 \tilde{\psi} = 0 \tag{2}$$

and

$$\left(1 + \frac{2\tilde{\varepsilon} De}{\tilde{\kappa}^2} \tilde{\tau}_{xy}^2\right) \tilde{\tau}_{xy} = \frac{\mathrm{d}\tilde{u}}{\mathrm{dY}} \tag{3}$$

Here $\tilde{\varepsilon}$ is a parameter that governs the extensional flow response, and the Debora number is defined as $De = \lambda_0 \kappa U_{HS}$ where λ_0 represents the relaxation time. Combining the equations (2) and (3) and integrating twice the equation of momentum in the Y direction using the symmetry boundary condition of the dimensionless velocity gradient, i.e., at $Y = 0$, $d\tilde{u}/dY = 0$ and the no-slip boundary condition at $Y = 1$, $\tilde{u} = 0$ and we obtain

$$\tilde{u} = \frac{d\tilde{P}}{d\chi}\left(\frac{Y^2-1}{2}\right) - \tilde{\zeta}\left(1 - \frac{\cosh\tilde{\kappa}Y}{\cosh\tilde{\kappa}}\right) + \frac{2\tilde{\varepsilon}De^2}{\tilde{\kappa}^2}\left\{\frac{1}{4}\left(\frac{d\tilde{P}}{d\chi}\right)^3 (Y^4 - 1) + 3\tilde{\kappa}\tilde{\zeta}\left(\frac{d\tilde{P}}{d\chi}\right)^2 \left[\frac{(\tilde{\kappa}^2+2)\cosh\tilde{\kappa} - 2\tilde{\kappa}\sinh\tilde{\kappa}}{\tilde{\kappa}^3\cosh\tilde{\kappa}} - \frac{(\tilde{\kappa}^2Y^2+2)\cosh\tilde{\kappa}Y - 2\tilde{\kappa}Y\sinh\tilde{\kappa}Y}{\tilde{\kappa}^3\cosh\tilde{\kappa}}\right] + 3\tilde{\kappa}^2\tilde{\zeta}^2\frac{d\tilde{P}}{d\chi} \left[\frac{2\tilde{\kappa}Y(\sinh 2\tilde{\kappa}Y - \tilde{\kappa}Y) - \cosh 2\tilde{\kappa}Y}{8\tilde{\kappa}^2\cosh^2\tilde{\kappa}} - \frac{2\tilde{\kappa}(\sinh 2\tilde{\kappa} - \tilde{\kappa}) - \cosh 2\tilde{\kappa}}{8\tilde{\kappa}^2\cosh^2\tilde{\kappa}}\right] + \tilde{\kappa}^3\tilde{\zeta}^3\left[\frac{\cosh 3\tilde{\kappa} - 9\cosh\tilde{\kappa}}{12\tilde{\kappa}\cosh^3\tilde{\kappa}} - \frac{\cosh 3\tilde{\kappa}Y - 9\cosh\tilde{\kappa}Y}{12\tilde{\kappa}\cosh^3\tilde{\kappa}}\right]\right\} \tag{4}$$

Here the dimensionless form of the varying wall zeta potential is $\tilde{\zeta}(x) = 1 + \varepsilon\sin 2\pi\chi$, where $\varepsilon = \Delta\zeta/\zeta_0$ is the dimensionless amplitude of the fluctuations of the alternating modulation component of the wall potential. Using the continuity equation and together with the impermeability boundary conditions at the upper and lower walls ($\tilde{v} = 0$ at $Y = \pm 1$) of the micro-channel, we obtained the equation for the dimensionless pressure gradient given as,

$$0 = -\frac{2}{3}\frac{d^2\tilde{P}}{d\chi^2} + 2\frac{d\tilde{\zeta}}{d\chi}\left(1 - \frac{\tanh\tilde{\kappa}}{\tilde{\kappa}}\right) + \frac{2\tilde{\varepsilon}De^2}{\tilde{\kappa}^2}\left\{-\frac{6}{5}\left(\frac{d\tilde{P}}{d\chi}\right)^2\frac{d^2\tilde{P}}{d\chi^2} + 3\tilde{\kappa}\left[2\tilde{\zeta}\frac{d\tilde{P}}{d\chi}\frac{d^2\tilde{P}}{d\chi^2} + \left(\frac{d\tilde{P}}{d\chi}\right)^2\frac{d\tilde{\zeta}}{d\chi}\right]\left[\frac{2\left(\tilde{\kappa}^2 - 2\tilde{\kappa}\tanh\tilde{\kappa} + 2\right)}{\tilde{\kappa}^3} - \frac{2\left(\tilde{\kappa}^2+6\right)\tanh\tilde{\kappa} - 8\tilde{\kappa}}{\tilde{\kappa}^4}\right] + 3\tilde{\kappa}^2\frac{d}{dx}\left[\tilde{\zeta}^2\frac{d^2\tilde{P}}{d\chi^2}\right]\left[\frac{\left(-2\tilde{\kappa}^3 - 3\sinh 2\tilde{\kappa} + 3\tilde{\kappa}\cosh 2\tilde{\kappa}\right)}{12\tilde{\kappa}^3\cosh^2\tilde{\kappa}} - \frac{2\tilde{\kappa}(\sinh 2\tilde{\kappa} - \tilde{\kappa}) - \cosh 2\tilde{\kappa}}{4\tilde{\kappa}^2\cosh^2\tilde{\kappa}}\right] + 3\tilde{\kappa}^3\tilde{\zeta}^2\frac{d\tilde{\zeta}}{d\chi}\left[\frac{\cosh 2\tilde{\kappa} - 5}{3\tilde{\kappa}\cosh^2\tilde{\kappa}} - \frac{\tanh\tilde{\kappa}\,(\cosh 2\tilde{\kappa} - 13)}{9\tilde{\kappa}^2\cosh^2\tilde{\kappa}}\right]\right\} \tag{5}$$

Integrating the velocity $\tilde{u}$ given in equation (4), from $Y = 0$ to $Y = 1$, the dimensionless volumetric flow rate $\tilde{Q}$, is represented by,

$$\tilde{Q} = -\frac{1}{3}\frac{d\tilde{P}}{d\chi} + \tilde{\zeta}\left(1 - \frac{\tanh\tilde{\kappa}}{\tilde{\kappa}}\right) + \frac{2\tilde{\varepsilon}De^2}{\tilde{\kappa}^2}\left\{-\frac{1}{5}\left(\frac{d\tilde{P}}{d\chi}\right)^3\right.$$
$$+3\tilde{\kappa}\tilde{\zeta}\left(\frac{d\tilde{P}}{d\chi}\right)^2\left[\frac{\tilde{\kappa}^2 - 2\,\tilde{\kappa}\sinh 2\tilde{\kappa} + 2}{\tilde{\kappa}^3} - \frac{(\tilde{\kappa}^2+6)\tanh\tilde{\kappa} - 4\tilde{\kappa}}{\tilde{\kappa}^4}\right] \tag{6}$$
$$+3\tilde{\kappa}^2\tilde{\zeta}^2\frac{d\tilde{P}}{d\chi}\left[\frac{3\tilde{\kappa}\cosh 2\tilde{\kappa} - 2\tilde{\kappa}^3 - 3\sinh 2\tilde{\kappa}}{24\tilde{\kappa}^3\cosh^2\tilde{\kappa}} - \frac{2\tilde{\kappa}(\sinh 2\tilde{\kappa} - \tilde{\kappa}) - \cosh 2\tilde{\kappa}}{8\tilde{\kappa}^2\cosh^2\tilde{\kappa}}\right]$$
$$\left.\tilde{\kappa}^3\tilde{\zeta}^3\left[\frac{\cosh 2\tilde{\kappa} - 5}{6\tilde{\kappa}\cosh^2\tilde{\kappa}} - \frac{(\sinh 2\tilde{\kappa} - 13)\tanh\tilde{\kappa}}{18\tilde{\kappa}^2\cosh^2\tilde{\kappa}}\right]\right\}$$

On the other hand, the Taylor-dispersion coefficient in dimensionless form can be written as follows [9],

$$\tilde{K}_{eff} = 1 + Pe^2\tilde{Q}^2\int_{Y=0}^{Y=1}\left[\int_{Y=0}^{Y=Y}\left(\frac{\tilde{u}}{\tilde{Q}} - 1\right)dY\right]^2 dY \tag{7}$$

In equation (7) the dimensionless dispersion coefficient is $\tilde{K}_{eff} = K_{eff}/D$, and the Péclet number is defined as $Pe = U_{HS}H/D$. Here D is the diffusion coefficient and K_{eff} represents the dispersion coefficient in physical units.

3. Results and Conclusions

We note that since $\tilde{P}(\chi)$ is unknown, the solution given in (4) and (6) are explicitly. In equation (4) is explicitly as a function of the dimensionless transversal coordinate Y and implicitly as a function of $d\tilde{P}/d\chi$. In equation (6) is implicitly as a function of χ through $d\tilde{P}/d\chi$. In this case to solve for of $d\tilde{P}/d\chi$, equation (5) was solved numerically using the shooting scheme. In this work, a $\Delta\chi$-step of 1×10^{-2} has been used in all numerical runs.

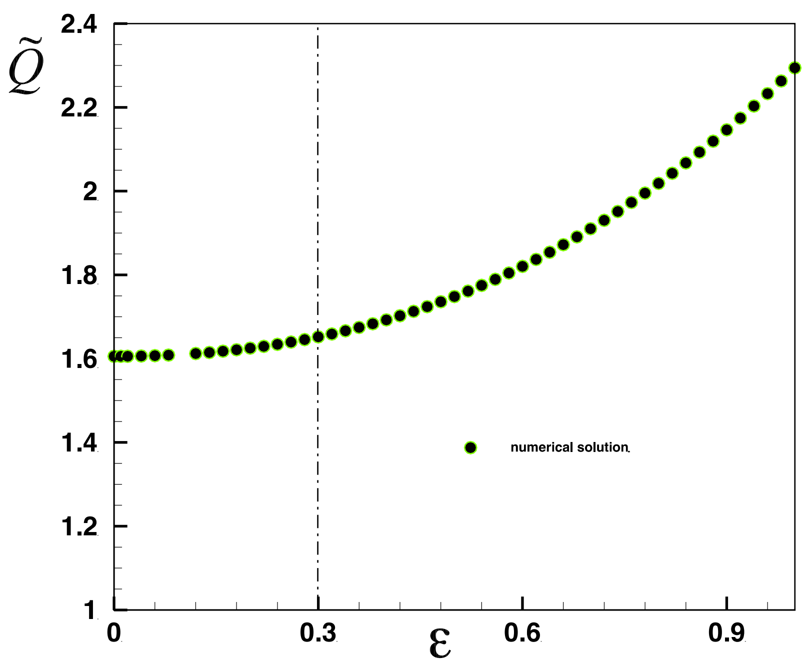

Fig. 2: Dimensionless flow rate as a function of the parameter ε with $\tilde{\varepsilon}De^2 = 1, \tilde{\kappa} = 20$; under the effect of a slowly variable wall potential $\tilde{\zeta}(\chi) = 1 + \varepsilon\sin 2\pi\chi$.

Figure 2 shows the variation of the dimensionless flow rate $\tilde{Q}$ under the influence of varying wall potential $\tilde{\zeta}$. The value of $\tilde{Q} = 1.6$, represents the well-known dimensionless flow rate for purely electroosmotic flow of a viscoelastic fluid with constant zeta-wall potential. When $\varepsilon > 0$ the volumetric flow rate changes increasing in non-linear form due to the combined effects of $\tilde{\zeta}$ and the induced pressure gradient $d\tilde{P}/d\chi$ in the dimensionless flow rate $\tilde{Q}$ as can be seen in equation (6).

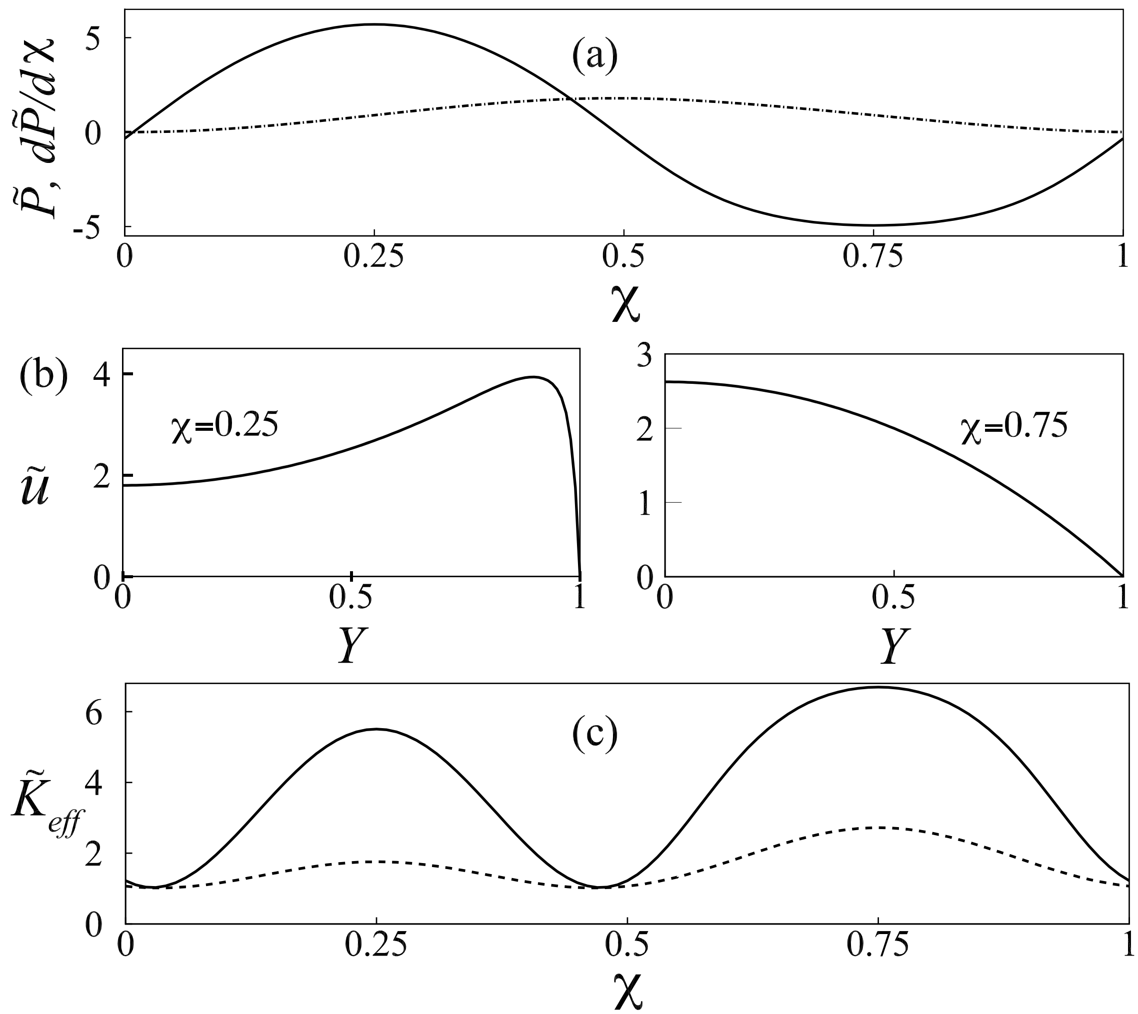

Fig. 3: Numerical solution of: dimensionless pressure (dash dot line) and pressure gradient (solid line) with $\tilde{\varepsilon}De^2 = 1$; (b) dimensionless velocity $\tilde{u}$ at selected values of χ with $\tilde{\varepsilon}De^2 = 1$; (c) variation of the effective dispersion coefficient $\tilde{K}_{eff}$ with axial position; caused by a varying wall potential $\tilde{\zeta}(\chi) = 1 + \varepsilon \sin 2\pi\chi$, where dashed line corresponds to $\tilde{\varepsilon}De^2 = 0$ and solid line to $\tilde{\varepsilon}De^2 = 1$ with $\varepsilon = 1$, $Pe = 10$ and $\tilde{\kappa} = 20$.

On the other hand, the 3(a) describes the behavior of a purely electroosmotic flow by imposing a sinusoidally varying zeta potential given by $\tilde{\zeta}(\chi) = 1 + \varepsilon \sin 2\pi\chi$. It is evident the strong influence of $\tilde{\zeta}$ in the hydrodynamics of the flow along the microchannel as it is shown in figure 3(a) we observe that from $0 < \chi \leq 0.5$ adverse pressure gradients are induced and contrariwise favorable pressure gradients are induced from $0.5 < \chi \leq 1$. In fact, at $\chi = 0.25$ and at $\chi = 0.75$, $\tilde{\zeta}$ has its maximum and minimum values at these positions the maximum values of the dimensionless induced pressure gradients as a function of $\tilde{\varepsilon}De^2$ and ε are obtained. As we can see in 3(b) the velocity $\tilde{u}$ is distorted exhibiting a concave profile over the cross-section. The concave effect is more pronounced and at the center of the micro-channel ($Y = 0$), the flow seems to have a retarding effect. For favorable dimensionless pressure gradient the profile of $\tilde{u}$ is distorted exhibiting a slightly convex behavior. The convex effect is more pronounced and at the center of the micro-channel ($Y = 0$), the flow seems to have an accelerated effect. In figure 3(c), equation (7) is plotted when the wall zeta potential $\tilde{\zeta}$ is modulated by means of the dimensionless amplitude ε the adverse and favorable pressure gradients and consequently the concave and convex shapes of the velocity profiles strongly distort the distribution of $\widetilde{K}_{eff}$ as is shown in figure 3(c). The dashed line in figure 3(c) represents the solution of the dispersion coefficient when the solvent and solute are considered as Newtonian fluids ($\tilde{\varepsilon}De^2 = 0$).

4. Conclusion

The dimensionless dispersion coefficient of a neutral non-reacting solute, in a steady pure EOF in a two-dimensional slit micro-channel, considering the combined effect of the viscoelasticity of the fluid and axial-modulations on the wall $\tilde{\zeta}$-potential, are analyzed theoretically herein. With the assumptions of the solute and solvent obey the sPTT constitutive equation, the associated governing equations for the fluid were simplified in the limit of the LAT and were solved numerically. Keeping in mind that the wall $\tilde{\zeta}$-potential varies periodically in the axial direction, the Poisson-Boltzmann equation was solved by considering non-overlapping EDLs and the Debye-Hückel approximation. Once the hydrodynamics were known, the axial distribution of the dispersion coefficients was determined as a function of the main parameters involved, $\tilde{\varepsilon}De^2$ and ε. With the results presented in this work and after having discussed them in detail, the following conclusions have been reached:

1.The varying $\tilde{\zeta}$-potential induces a dimensionless pressure gradient that varies periodically in the axial direction. The axial distribution in the adverse and favorable regions of the dimensionless pressure gradient becomes increasingly amplified with the dimensionless amplitude of the fluctuations ε.

2.The velocity profiles across the channel-width become concave at region where $\tilde{\zeta} > 1$ and parabolic at region where $\tilde{\zeta} < 1$. The velocity gradients in both region are then controlled by the dimensionless amplitude of the fluctuations ε, which might then induce a stronger non-periodical dispersion in the axial direction.

3.The local and global maximum values of the dispersion coefficient $\widetilde{K}_{eff}$, are located at positions at which $d\tilde{P}/d\chi$ is zero, then concave and parabolic velocity profiles at these positions are developed; causing a global maximum value of $\widetilde{K}_{eff}$ in the region where the velocity has a parabolic form.

4.For $\tilde{\varepsilon}De^2 = 1$ and $\varepsilon = 1$ and considering that $\tilde{\zeta}$ takes the form $\tilde{\zeta}(\chi) = 1 + \varepsilon \sin 2\pi\chi$, there is an increment of about 158% in the local value of $\widetilde{K}_{eff}$ in comparison with that obtained when the solute and the solvent are assumed to be Newtonian fluids ($\tilde{\varepsilon}De^2 = 0$). Then viscoelastic effects under this condition can be well considered for improving the dispersion coefficient.

5.The dimensionless flow rate $\tilde{Q}$ for the electroosmotic flow of a sPTT fluid with constant $\tilde{\zeta}$-potential was increased in about 43.75%, when $\varepsilon = 1$ and $\tilde{\varepsilon}De^2 = 1$ were considered.

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