

Gel electrophoresis and size selectivity of charged colloidal particles in a charged hydrogel medium



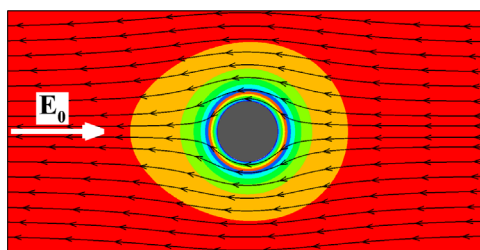
S. Bhattacharyya*, Simanta De

Department of Mathematics, Indian Institute of Technology Kharagpur, Kharagpur-721302, India

HIGHLIGHTS

- Numerical study based on the Stokes–Nernst–Planck–Poisson equations.
- Impact of double layer polarization and convective transport of ions.
- Background EOF drags the negatively charged particle along the imposed electric field.
- Size-selectivity in a highly charged gel medium is demonstrated.

GRAPHICAL ABSTRACT



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ABSTRACT

The electrophoresis of a charged colloid particle embedded in a charged hydrogel medium is studied based on the numerical computation of Stokes–Nernst–Planck–Poisson equations. In this study, no prior assumption on surface charge density of the particle, Debye length and imposed external electric field are made. We have compared our computed results for a lower range of surface charge density with the existing analytical solution based on the weakly charged particle and found them in good agreement when the fixed charge density of the hydrogel is low. Nonlinearity effects in gel electrophoresis is pronounced for a thick Debye length and higher values of particle ζ -potential. Even in the absence of a gel medium (free-solution), the numerical procedure used in this work yields mobilities different from the previous theoretical analysis based on the Debye–Hückel approximation when the scaled ζ -potential exceeds 2 and the Debye length is in the order of the particle size. The strong background electroosmotic flow (EOF) for a high fixed charge density of the polyelectrolyte hydrogel with a mesh size comparable to the particle radius drags the particle along the direction of the EOF. In this case, the electrophoretic velocity of the particle varies with its size. The particle electrophoretic velocity and forces are determined for a wide range of intrinsic parameters values.

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1. Introduction

Hydrogels are water-saturated cross-linked polymers having a porous structure with molecular-scale porosity. Electrophoresis in hydrogel medium is widely used to separate biomolecules such as DNA and proteins in electrophoretic applications (Görg, 1994; Yoshioka et al., 2003). Electrokinetic transport in a permeable

membrane with charged inclusions has importance in the context of biological cells, dialysis and fuel cells (Hill, 2006). Gel electrophoresis is also important in remediating a contamination in situ (Jones et al., 2011). The widespread applications of gel electrophoresis and its advantages over the conventional free electrophoresis in a liquid medium has already been discussed in several articles e.g., Li and Hill (2013), Bhattacharyya et al. (2014).

Gel electrophoresis is complicated compared to free electrophoresis due to the occurrence of long range hydrodynamic interactions and short range steric effects on account of friction between the gel skeleton and the particles. The long range effects

* Corresponding author.

E-mail addresses: somnath@maths.iitkgp.ernet.in (S. Bhattacharyya), simanta.de@gmail.com (S. De).

can be modeled through the effective medium approach (Johnson et al., 1996), in which the hydrogel is modeled as a continuum and the hydrodynamics is governed by the Brinkmann equation. If the particle size is comparable to the gel mesh size then the steric interaction becomes important. Brady (1994) proposed that the diffusivity in a gel can be expressed as a product of factors which accounts for the hydrodynamic effect and the steric effect. This model was validated experimentally, theoretically and computationally by several authors namely, Johansson and Löfroth (1993), Allison et al. (2007), Tsai et al. (2011) and Hsu et al. (2012). Doane et al. (2010) introduced a frictional coupling force to model the steric interactions between the particle and the hydrogel skeleton.

Based on the effective medium approach, the long range interactions in gel electrophoresis have been addressed by several authors namely, Hill (2006), Allison et al. (2007), Tsai et al. (2011), Tsai and Lee (2011), Hsu et al. (2012), Hsu et al. (2013) and Bhattacharyya et al. (2014). When the electrostatic force and hydrodynamic drag experienced by the particle is balanced then the particle migrates at a constant velocity; the electrophoretic velocity. Allison et al. (2007) provided an analytical formulae to determine the electrophoretic mobility of a particle with low and high surface charge. The double layer polarization (DLP) effects on mobility has been analyzed by Tsai et al. (2011) based on a first-order perturbation analysis. Hsu et al. (2012) found through the first-order perturbation analysis under a weak field assumption that the DLP effect in gel electrophoresis is low compared to the free-solution electrophoresis and it is further diminished with the increase of gel concentration. Recently, Bhattacharyya et al. (2014) determined the mobility and forces and validated the formulae of Allison et al. (2007) by considering the double layer polarization effects. There it was found that the double layer polarization and relaxation effect in uncharged electrophoresis is significant when the particle is highly charged and the gel is highly permeable.

Agarose gel has been used for gel electrophoresis because of its favorable permeability. Many hydrogels e.g., agarose gel are charged or acquire charges due to chemical reactions (Li and Hill, 2013 and the references there-in). In presence of an electric field, the mobile counterions in gel get transported towards the oppositely charged electrodes and therefore induce an electroosmotic flow (EOF). This EOF affects the electrophoretic transport of a charged particle. Mohammadi and Hill (2010) analyzed the electrokinetic transport of uncharged inclusions in a charged hydrogel due to the impact of electroosmotic flow theoretically. The size selectivity of nanoparticles coated with a charged polymer layer in gel electrophoresis was demonstrated experimentally by Hanauer et al. (2007). Doane et al. (2010) made experimental and theoretical studies to quantify the mobility of weakly charged PEGylated metal nanoparticles in a charged hydrogel medium. Subsequently, Li and Hill (2013) extended this study for weakly charged bare nanoparticles in a charged or uncharged hydrogel. There they obtained an expression by modifying the theory of Allison et al. (2007) for determining the mobility of a charged particle in a charged hydrogel medium. The electrophoresis of soft particles in polyelectrolyte hydrogels is studied under the Debye–Hückel approximation by Li et al. (2014). Li et al. (2014) have shown that the dielectric permittivity of the particle has an impact on gel electrophoresis. Their analysis shows that the DLP effect diminishes the magnitude of the mobility. It has been predicted in that paper that the double layer polarization and relaxation have a strong impact for a metallic particle (large dielectric permittivity), but these effects are negligible at a thin Debye length for a perfectly dielectric particle (zero permittivity). It may be noted that for a soft particle, as considered by Li et al. (2014), the nonlinear effects such as DLP and relaxation become less important as compared to a bare particle. A similar problem, as considered by Doane et al. (2010) and Li et al. (2014), is analyzed through a different approach by Allison et al. (2014).

In this paper, we have considered the electrophoresis of a charged particle in a charged hydrogel medium. Our analysis is based on the computation of the coupled Stokes–Nernst–Planck–Poisson equations in their full form. The numerical study based on the computation of the Nernst–Planck equations for ion transport on colloid dispersions is rather limited owing to its several complexities. Recently, Shih and Yamamoto (2014) performed direct numerical simulations to study the electrokinetics of charged colloids in an AC electric field. We developed the computer code, which we have validated by comparing with several experimental and theoretical solutions. The mechanism of electrokinetic transport of a nanoparticle in a charged hydrogel is studied by considering the interactions of electroosmosis, double layer polarization (DLP), hydrodynamic drag and electrostatic force. We have highlighted the impact of the double layer polarization and interaction of the background EOF on gel electrophoresis by comparing with the existing analytical solutions. The present analysis does not consider the steric interactions with the gel skeleton. One of the objectives of the present study is to demonstrate the size selectivity of nanoparticles by electrophoresis in a charged hydrogel medium. Our results show that by suitably tuning the fixed charge density of the hydrogel and ionic concentration of added electrolyte, a size-selectivity can be achieved.

2. Mathematical model

We consider the electrophoresis of a nonconductive, impermeable charged spherical particle of radius a in a charged hydrogel under an applied electric field E_0 . In presence of the applied electric field, the particle moves with a constant velocity U_E^* relative to the surrounding medium. This problem is equivalent to that of a stationary sphere experiencing an incoming flow at a uniform velocity of $-U_E^*$ far from the particle surface in a frame of reference fixed at the center of the particle (Fig. 1(a)). A spherical polar coordinate (r, θ, ψ) is adopted with the origin at the center of the sphere and the initial line ($\theta = 0$) is the z -axis along which the electric field is imposed. We assume that the problem to be axially symmetric with z -axis as the axis of symmetry.

The hydrogel is modeled as a Brinkman medium with screening length ℓ , which characterize the hydrodynamic permeability of the medium. We consider a uniformly charged hydrogel skeleton with fixed charge density ρ_f which is of the same sign as that of the surface charge density of the particle. The equations governing this electrokinetic phenomena are the Darcy–Brinkman extended Stokes equation with electric body force term for fluid flow, the Nernst–Planck equations for ion transport, and the Poisson equation for the electric field. For simplicity, we have considered a symmetric z - z electrolyte with valance $z_i = \pm \mathcal{Z}$ for $i = 1, 2$, respectively. Following Saville (1977), we have scaled the variables as follows. The radius of the sphere a is considered as the length scale, the thermal potential $\phi_0 = k_B T / \mathcal{Z} e$ is the potential scale, $U_0 = (\epsilon_e \phi_0^2 / \mu a)$ is the velocity scale, $\epsilon_e \phi_0^2 / a^2$ is the pressure scale and the bulk ionic number n_i^0 is the scale for ionic concentration. Here e is the elementary electric charge, k_B is the Boltzmann constant, T is the absolute temperature, ϵ_e is the permittivity of the medium and μ is the viscosity. The velocity scale U_0 corresponds to the Smoluchowski velocity for surface potential ϕ_0 under an electric field ϕ_0/a . The non-dimensional parameter $\beta = a/\ell$ provides a measure of the permeability of the gel medium. A higher value of β implies a lower permeability of the gel medium. Here $\kappa_s = \sqrt{2 \mathcal{Z} I_0 e / \epsilon_e \phi_0}$ is the inverse of the EDL thickness based on the bulk concentration I_0 of the added electrolyte. The non-dimensional form of the Stokes–Brinkman equations for Newtonian fluid to describing the motion of ionized fluid in uniformly charged

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