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A generalised model for electro-osmotic flow in porous media

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A generalised model for electro-osmotic flow in porous media

Abstract

Purpose - This work aims at developing a comprehensive model for the analysis of Electro-Osmotic Flow (EOF) through a fluid saturated porous medium. In order to fully understand and exploit a number of applications, such a model for EOF through porous media is essential.

Design/methodology/approach - The proposed model is based on a generalised set of governing equations used for modelling flow through fluid saturated porous media. These equations are modified to incorporate appropriate modifications to represent electro-osmosis. The model is solved through the Finite Element Method (FEM). The validity of the proposed numerical model is demonstrated by comparing the numerical results of internal potential and velocity distribution with corresponding analytical expressions. The model introduced is also used to carry out a sensitivity analysis of the main parameters that control electro-osmotic flow.

Findings - The analysis carried out confirms that electro-osmosis in free channels without porous obstructions is effective only at small scales, as largely discussed in the available literature. Employing porous media makes electro-osmosis independent of the channel scale. Indeed, as the channel size increases, the presence of the charged porous medium is essential to induce fluid flow. Moreover, results demonstrate that flow is significantly affected by the characteristics of the porous medium, such as particle size, and by the zeta potential acting on the charged surfaces.

Originality/value - To the best of author's knowledge, a comprehensive FEM model, based on the generalised equations to simulate electro-osmotic flow in porous media, is proposed here for the first time.

Paper type - Research paper

Keywords: Electro-osmosis; Porous media; Charged particles; Generalised model; Fractional step method

1 Introduction

Electro-Osmosis (EO) in porous media has been studied for over two centuries, due to its wide range of interests in civil, medical and industrial applications. It is employed for cooling of electronic devices (Berrouche

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et al., 2009; Cheema et al., 2013), dehumidification, dehydration and regeneration processes of solid desiccant in heating ventilation air conditioning systems (Li et al., 2013a,b), fabrication of micro biomedical technologies (Cheema et al., 2013; Misra and Chandra, 2013), treatments for environmental purposes (Li et al., 2013b; Hlushkou et al., 2005; Shapiro and Probst, 1993; Wu and Papadopoulos, 2000; Tallarek et al., 2002; Cameselle, 2015), dewatering (Lewis and Garner, 1972; Lewis and Humpheson, 1973), energy production (Cheema et al., 2013; Chen et al., 2014; Bennacer et al., 2007; Mahmud Hasan et al., 2011). In order to understand the physical phenomenon of EO, the concept of Electric Double Layer (EDL) needs to be introduced. A charged surface in contact with an electrolytic solution is usually deprotonated. Since the solid-liquid interface is negatively charged, it attracts the fluid cations that form a high concentration region, called EDL. As the distance from the charged surface increases, the ions concentration decreases and it can be considered equal to that of the bulk solution. The EDL is the main responsible for EO. When the distance from the charged surface is large compared to the EDL thickness, the velocity is independent of the channel width and constant within the channel. For this reason, EO driven flow systems are mainly related to thin EDLs on charged surfaces. In other words, as the surface to volume ratio increases, Electro-Osmotic Flow (EOF) increases. Therefore, unlike pressure driven flow, where velocity is proportional to the square of the channel width, EO is more effective at micro-scale. In fluid systems, only the channel walls can be considered as electrically active surfaces. When charged solid particles are introduced inside a channel, their surface will also influence the EOF. As a consequence, porous electro-osmotic systems are getting more and more attractive. Indeed in low porosity media, EOF has been found to be effective (Anderson and Keith Idol, 1985) and more advantageous than pressure-driven flows (Hlushkou et al., 2005; Tallarek et al., 2002).

One of the first applications for EOF in porous media has been Capillary ElectroChromatography (CEC), where electro-osmosis is used to drive flow in packed capillary columns (Hlushkou et al., 2005; Tallarek et al., 2002; Rathore and Horváth, 1997; Li and Remcho, 1997; Wan, 1997; Liapis and Grimes, 2000; Hlushkou et al., 2006), instead of hydrostatic pressure as in classical high-performance liquid chromatography systems. While analysing such systems, several parameters are found to influence EOF in porous media. The velocity increases as the applied electrical field increases (Liapis and Grimes, 2000). Also, the wall zeta potential affects the flow, but only within about one third of the capillary radius (Rathore and Horváth, 1997; Liapis and Grimes, 2000). The velocity decreases as the particle diameter increases, with more significant effects noticed at higher differences between the zeta potential of the walls and that of the particles (Liapis and Grimes, 2000). Also, the orientation and contact of fibres in arrays of ordered fibrous porous media (Kozak and Davis, 1986), the concentration and distance of solid particles (Kozak and Davis, 1989; Di Fraia et al., 2017) and the connectivity among the intra-particle pores (Grimes et al., 2000) influence EOF.

Beyond CEC, EO is commonly used for micro-pumping. The analysis in such systems is carried out mainly through analytical models, focused on the maximum pressure, maximum flow rate and efficiency of the pump. The first theory has been introduced by Zeng et al. (2001), and then used as it is or extended by other authors. Yao and Santiago (2003) modified this model, considering two terms composing the total current, the advective and the electromigration currents. The analytical model proposed by Zeng et al. has been used to examine a high-pressure EO micro-pump (Wang et al., 2006) or to compare two types of porous

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ceramics, sintered alumina and silica, to realize an EO pump (Berrouche et al., 2009). The studies on EO pumps highlight the influence on EOF of pore radius and porosity (Berrouche et al., 2009; Cheema et al., 2013; Yao et al., 2006).

In general, porous medium flow can be studied by using several approximations and assumptions. Depending on the chosen approach, fluid flow in porous media can be investigated at the pore level or by using a macroscopic method. Obviously, the first approach provides minute details of flow, but it is computationally expensive (Massarotti et al., 2003). For this reason, such a method is only employed when the interaction mechanisms at the internal interfaces between the materials that compose the porous medium, need to be accurately determined (Ehlers and Bluhm, 2013). The flow in a homogeneous porous medium can be analysed as a continuum through an appropriate averaging process (Ehlers and Bluhm, 2013), which can be:

- statistical, if the porous medium is averaged over reference porous structures, by assuming a statistical homogeneity;
- spatial, by averaging the medium over the so-called Representative Elementary Volume (REV) (Whitaker, 1967), whose scale, l , is larger than the scale of the porous medium particle, d_p , and smaller than that of the flow domain, L (Nield and Bejan, 2006), as shown in Figure 1.

The basic law governing fluid flow through porous media is Darcy's equation, which linearly relates the pressure gradient to the flow rate across the porous medium (Darcy, 1856). To overcome the limitations of the Darcy theory, several *non-Darcy models* have been introduced. The most common are:

- Forchheimer's equation (Forchheimer, 1901), needed at high velocity to model the drag effect on the fluid due to the solid matrix;
- Brinkman extension (Brinkman, 1949), to take into account macroscopic boundary effects.

The Darcy equation and its extensions have been incorporated in the so-called generalized porous medium

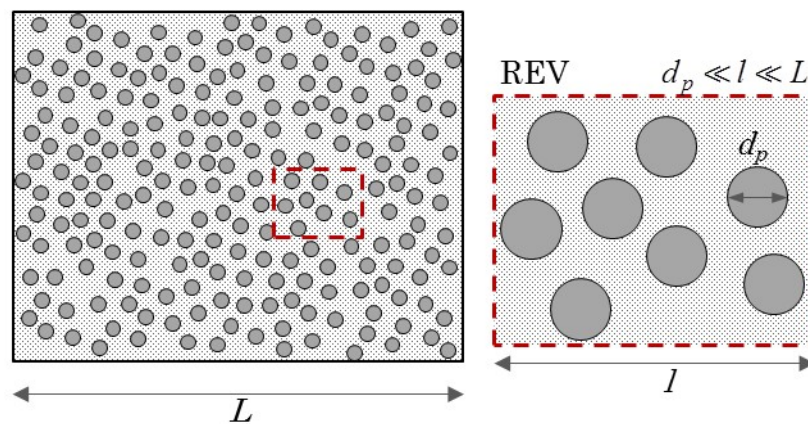


Figure 1: Representative Elementary Volume (REV) and scales in macroscopic approach to model flow in porous media.

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65 model, firstly introduced by Whitaker (1967). This author proposed a volume averaging procedure, later
66 used by Vafai and Tien (1981) and Hsu and Cheng (1990). Based on Whitaker's method, a control volume
67 principle was developed by Nithiarasu et al. (1996) to take into account the variability of porosity in satu-
68 rated porous media. This generalised model is based on the classical Navier-Stokes equations, to which it
69 approaches when the porosity approaches unity and the permeability tends to infinity.

1.1 Generalized model for porous media in EO

71 The generalized model for flow through porous media has been used for the first time to investigate EO by
72 Scales and Tait (2006). By using the Navier-Stokes equations, properly averaged to compute flow through
73 porous media (Vafai and Tien, 1981; Liu and Masliyah, 1996; Nithiarasu et al., 1997), they developed a
74 model to describe EO and pressure driven flow in porous media. They introduced an additional term to
75 take into account the effect of charged solid particles, the so-called effective charge density, ρ_{eff} , dependent
76 on the properties of the porous medium. Assuming several simplifying assumptions, they developed the
77 analytical solutions for EOF in porous media for simple geometrical configurations. Kang et al. (2004a)
78 employed the Carman-Kozeny theory (Probstein, 2005) to study Alternating Current (AC) driven EO sys-
79 tems in closed-end micro-channels densely packed with uniform charged spherical micro-particles. They
80 analytically solved the Poisson-Boltzmann equation to derive the internal potential, implemented as a source
81 term in the fluid motion equation. Then they analytically solved the modified Brinkman momentum equa-
82 tion, to calculate the back pressure due to a fixed excitation frequency. As a characteristic length, they used
83 the hydraulic diameter or effective pore diameter. EOF due to AC presents a harmonic sinusoidal oscillation.
84 The oscillating Darcy velocity profile is affected by pore size and excitation frequency. The model devel-
85 oped is validated against experimental results and used to test the effect of several parameters on EOF (Kang
86 et al., 2007). The factors with the largest influence are the ionic concentration and the type of electrolyte,
87 due to their impact on the zeta potential magnitude. On the contrary, the capillary length has a negligible
88 influence. Wall effect is more significant as the ratio between the capillary diameter and the particle diame-
89 ter decreases. The model has been further extended (Kang et al., 2004b) by distinguishing the contribution
90 from the charged capillary wall and that from charged particles. In the case of neutral packing particles,
91 macroscopic EOF is determined through the Brinkman momentum equation. This latter is modified by im-
92 plementing the internal potential, introduced as an analytical solution of the Poisson-Boltzmann equation,
93 with channel width used as the reference length. Through this model, Kang et al. (2005) investigated the
94 influence on EOF of the properties of both the working fluid and the porous medium. The effect of charged
95 walls is considerable only in case of similar size of the particles and the micro-capillary. The authors also
96 analysed the effect of the difference between the charge of the wall and that of the particles, founding similar
97 results to those of Liapis and Grimes (2000).

98 EOF in porous media has been investigated by using the Carman-Kozeny model also by Chai et al. (2007).
99 In particular, they solved the generalized porous medium equations proposed by Nithiarasu et al. (1997)
100 through the Lattice-Boltzmann Method (LBM). They modified the momentum equation to take into account
101 the EO effect by implementing the net charge density, ρ_e , and the effective charge density, ρ_{eff} , into the

102 source term, as proposed by Scales and Tait (2006). The linearized Poisson-Boltzmann equation, averaged
103 through the tortuosity of the porous medium, is used to determine the internal potential. They simulated a
104 micro-channel filled with a solid medium with varying porosity at several operating conditions: generally
105 velocity increases with the applied electric field and the porosity, and decreases as the tortuosity increases,
106 due to the consequent permeability reduction. It also increases with particle size, probably as a consequence
107 of the porosity increase. For larger particle sizes another effect is enhanced: the drag action due to the
108 porous medium prevents the viscous transfer of momentum from the channel walls to the centre of the
109 channel. The velocity near the walls is higher in the case of variable porosity with respect to the condition of
110 constant porosity. As a consequence, porosity variability in the region close to the walls cannot be neglected,
111 confirming the results reported by Cheema et al. (2013).

112 Recently, the use of non-Newtonian fluids, such as bio-fluids, in EO driven systems is increasing. The
113 generalised model proposed by Nithiarasu et al. (1997) has been used by Tang et al. (2010) to develop a
114 LBM model on the REV scale for EO and pressure driven flow in porous media, with non-Newtonian fluids.
115 Two source terms are added to the momentum equations: one to introduce the flow resistance due to the flow
116 of Non Newtonian fluids in porous media (Herschel and Bulkley, 1926; Al-Fariss and Pinder, 1987) and the
117 other for the electro-kinetic effect. For the EO contribution, charged solid particles and charged channel
118 walls are considered. An effective charge is used to take into account the contribution of porous medium
119 on EOF. A low value of zeta potential is assumed in order to use Debye-Hückel simplification and linearise
120 the Poisson-Boltzmann equation for internal potential computation. A modified zeta potential is considered
121 as a boundary condition to account for the influence of charged solid particles on the internal potential
122 distribution between the parallel walls of the channel. The model developed has been solved through LBM
123 and used to assess the influence of several parameters on EOF. Concerning flow resistance due to the use
124 of non-Newtonian fluids, the velocity increases with decreasing power law exponent and yield stress, and
125 increasing solid particle diameter and porosity. The influence of the channel wall zeta potential is significant
126 close to the wall, whereas the zeta potential of solid particles affects velocity in the central region of the
127 channel.

128 *1.2 Aim of the work*

129 The analysis of available literature on EOF through porous media has highlighted that the existing ap-
130 proaches and models focus on different aspects and that many simplifying assumptions are still used, re-
131 garding both electrical field and fluid flow equations (Di Fraia et al., 2018). For this reason, in this work a
132 generalised model is proposed to predict electro-osmotic flow in porous media. As mentioned in the anal-
133 ysis of the state of art (See Section 1), the generalised porous media model has been employed by other
134 authors, especially to derive the analytical solution of simple configurations (Scales and Tait, 2006; Kang
135 et al., 2004a). The computational works in this area appear to have neglected the charge of solid particle
136 inside the porous medium (Kang et al., 2004b, 2005) or ignored the effect of non-linear drag force (the
137 Forchheimer's term in the momentum equation) (Chai et al., 2007).

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3 138 The proposed model addresses EOF in a comprehensive fashion by
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5 139 • accounting for the charge of both walls and solid particles;
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7 140 • including the drag effect on the fluid due to the solid matrix;
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9 141 • considering the macroscopic boundary effects;
10
11 142 • solving the equations using the Finite Element Method (FEM).

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13 143 To the best of author's knowledge, a comprehensive FEM model, based on the generalised equations to
14 144 simulate electro-osmotic flow in porous media is proposed here for the first time. The paper is organised
15 145 into the following sections. In Section 2 the governing equations of the developed model are introduced.
16 146 In Section 3, after its verification, the proposed model is used to assess the effectiveness of using porous
17 147 media to enhance EOF by comparing the results obtained for free channels and channels packed with porous
18 148 media. Since the literature review has highlighted that many parameters can affect EOF, such comparison
19 149 is carried out by analysing the influence of channel width, particle size, zeta potential of charged particles
20 150 and bulk ionic concentration of the electrolyte. Finally, in Section 4, the main conclusions of the work are
21 151 drawn.

152 2 Mathematical model and solution procedure

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30 153 As explained in Section 1, the electric field responsible for EOF is induced by the interaction between an
31 154 external applied potential and the EDL. The electrokinetic forces responsible for EOF are modelled through
32 155 a Laplace equation governing the externally applied potential and a Poisson-Boltzmann equation governing
33 156 the EDL potential. Their effect on the flow is taken into account through a source term in the momentum
34 157 equation (Patankar and Hu, 1998; Yang and Li, 1998). EOF through porous media is simulated by properly
35 158 modifying the generalised model for porous media introduced by Nithiarasu et al. (1997) to take into account
36 159 the charge of both channel walls and porous medium. As mentioned above, this generalised model is based
37 160 on the classical Navier-Stokes equations, to which it approaches when the porosity approaches unity, and
38 161 permeability tends to infinity. The equations for EOF are temporally discretized by using the Characteristic
39 162 Based Split (CBS) algorithm (Nithiarasu, 2003; Nithiarasu et al., 2016), while the Galerkin approximation
40 163 is used for spatial discretization.

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46 164 The proposed model is based on the following assumptions:

- 47 165 • 2D modelling, with flat surfaces, characterized by uniform charge along their length;
 - 48 166 • Boltzmann distribution for the ions inside the electrolyte;
 - 49 167 • constant properties of the electrolyte;
 - 50 168 • incompressible fluid;
 - 51 169 • constant porosity;
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- 170 • steady and fully developed flow.

171 2.1 Governing equations

172 The external potential ϕ is governed by a Laplace equation of the type:

$$\sigma_p \frac{\partial^2 \phi}{\partial x_i^2} = 0 \quad (1)$$

173 where σ_p is the electrical conductivity of porous medium particles. The external electric field, E_x , and the
174 external electric potential, ϕ , are related via

$$E_x = -\frac{\partial \phi}{\partial x_i} \quad (2)$$

175 The EDL potential, ψ , is described by a Poisson-Boltzmann equation, as follows:

$$\frac{\partial^2 \psi}{\partial x_i^2} = -\frac{\rho_e}{\epsilon \epsilon_0} \quad (3)$$

176 where ϵ is the dielectric constant of the electrolyte, ϵ_0 is the permittivity of vacuum and ρ_e is the net charge
177 density.

178 The equilibrium Boltzmann distribution equation can be used to predict the ionic number concentration
179 in the case of fully developed flow with small Peclet numbers (Yang et al., 2001) and in the absence of
180 overlapping of EDLs (Qu and Li, 2000). The ions in the solution are assumed to be equal but opposite in
181 charge, and they are related to their energy ($ze\psi$) as

$$n^+ = n_0 \exp\left(-\frac{ze\psi}{k_{Bo}T}\right); \quad n^- = n_0 \exp\left(\frac{ze\psi}{k_{Bo}T}\right); \quad (4)$$

182 where n^+ and n^- represent the number of positive and negative ions, respectively, n_0 is the ionic num-
183 ber concentration in the bulk solution, z is the valance of the ions, e is the elementary charge, k_{Bo} is the
184 Boltzmann's constant and T is the temperature in kelvin. The bulk ionic concentration n_0 can be obtained as

$$n_0 = cN_A \quad (5)$$

185 where c is the concentration of the electrolyte in Moles and N_A is Avogadro constant. Therefore, the net
186 charge density can be defined as

$$\rho_e = ze(n^+ - n^-) \quad (6)$$

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Using hyperbolic functions, the net charge density can be expressed as

$$\rho_e = -2n_0ze \sinh\left(\frac{ze\psi}{k_{Bo}T}\right) \quad (7)$$

The non-linear Poisson-Boltzmann equation, obtained by substituting Equation 7 into Equation 3, allows to determine the internal potential distribution of the ions inside the fluid as

$$\frac{\partial^2\psi}{\partial x_i^2} = \frac{2n_0ze}{\epsilon\epsilon_0} \sinh\left(\frac{ze\psi}{k_{Bo}T}\right) \quad (8)$$

Fluid flow phenomena through porous media due to EO is modelled by using the modified generalised model for porous media, that can be written as follows.

• Continuity equation

$$\frac{\partial\rho_f}{\partial t} + \rho_f \frac{\partial\bar{u}_i}{\partial x_i} = 0 \quad (9)$$

where ρ_f the fluid density, and \bar{u}_i is the volume averaged velocity defined as a function of the fluid velocity, u_i , $\bar{u}_i = \Phi u_i$, in which Φ is the medium porosity. By using the ideal gas law, the speed of sound c can be expressed as

$$c^2 = \frac{\partial p}{\partial\rho_f} \quad (10)$$

where p is the pressure. The continuity equation can be rewritten as follows

$$\frac{1}{c^2} \frac{\partial p}{\partial t} = -\rho_f \frac{\partial\bar{u}_i}{\partial x_i} \quad (11)$$

For incompressible flows, the speed of sound may be replaced with an artificial compressibility parameter β , (Nithiarasu, 2003).

• Momentum equation

$$\frac{\rho_f}{\Phi} \left(\frac{\partial\bar{u}_i}{\partial t} + \frac{\partial}{\partial x_j} \left(\frac{\bar{u}_i\bar{u}_j}{\Phi} \right) \right) = -\frac{1}{\Phi} \frac{\partial\Phi p}{\partial x_i} + \frac{\mu_{eff}}{\Phi} \frac{\partial^2\bar{u}_i}{\partial x_i^2} - \frac{\mu_f}{K} u_i - \rho_f \frac{c_F}{\sqrt{K}} |\mathbf{V}| \bar{u}_i + \Phi(\rho_e + \rho_{eff}) E_x \quad (12)$$

where μ_{eff} is the effective viscosity, used to take into account the viscous effect that increases as porosity and permeability increase (Massarotti et al., 2003), μ_f is the fluid viscosity, \mathbf{V} is the velocity vector in the

porous medium. The medium permeability K takes the well-known form of (Vafai, 2005)

$$K = \frac{\Phi^3 d_p^2}{b(1-\Phi)^2} \quad (13)$$

and the Forchheimer coefficient c_F is given as (Ergun and Orning, 1949)

$$c_F = \frac{b}{\sqrt{d\Phi^3}} \quad (14)$$

where constants b and d ($b = 150, d = 1.75$) depend on the microscopic geometry of the porous medium and d_p is the particle size of the bed.

The last term of Equation (12) takes into account the driving force of EOF due to the interaction between the EDL potential of both channel walls and particles composing the porous medium, and the external electric field. The effective charge density, ρ_{eff} , is added to the net charge density, ρ_e , in the source term, as proposed by Tang et al. (2010). Considering a cylindrical pore, an analytical expression may be expressed for effective charge density as (Tang et al., 2010):

$$\rho_{eff} = \frac{\Phi \epsilon \epsilon_0 \zeta_p}{K} \left(\frac{2I_1(\kappa R_{pore})}{\kappa R_{pore} I_0(\kappa R_{pore})} - 1 \right) \quad (15)$$

where I_n is the modified Bessel function of the first type of order n and R_{pore} is the average pore size calculated as

$$R_{pore} = \frac{d_p \Phi}{3(1-\Phi)} \quad (16)$$

The generalised model equations (Equations (11) and (12)) discussed above reduce to the Navier Stokes equations when the solid matrix in the porous medium disappears, i.e. when Φ tends to 1. Writing Equation (12) as

$$\frac{\rho_f}{\Phi} \left(\frac{\partial \bar{u}_i}{\partial t} + \frac{\partial}{\partial x_j} \left(\frac{\bar{u}_i \bar{u}_j}{\Phi} \right) \right) = -\frac{1}{\Phi} \frac{\partial \Phi p}{\partial x_i} + \frac{\mu_{eff}}{\Phi} \frac{\partial^2 \bar{u}_i}{\partial x_i^2} - P \quad (17)$$

where

$$P = \frac{\mu_f}{K} u_i + \rho_f \frac{c_F}{\sqrt{K}} |\mathbf{V}| \bar{u}_i + \Phi (\rho_e + \rho_{eff}) E_x \quad (18)$$

the same set of equations described above can be used to analyse the case of single-phase fluid, by assuming that the porosity is 1 and the term P is 0.

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2.1.1 Dimensionless form of the governing equations

For a homogeneous medium, with constant, uniform porosity and constant properties, the dimensionless form of the governing equations described above can be obtained through the following non-dimensional scales:

$$x_i^* = \frac{x_i}{L_{ref}}; \quad \phi^* = \frac{ze\phi}{k_{Bo}T}; \quad \psi^* = \frac{ze\psi}{k_{Bo}T}; \quad \rho^* = \frac{\rho_f}{\rho_{ref}}; \quad u_i^* = \frac{u_i}{u_{ref}};$$

$$u_{ref} = \frac{E_x \epsilon \epsilon_0 \zeta}{\mu_f}; \quad t^* = \frac{tu_{ref}}{L_{ref}}; \quad p^* = \frac{p - p_{ref}}{\rho_{ref} u_{ref}^2}; \quad \sigma^* = \frac{\sigma}{\sigma_{ref}}$$

where the subscript *ref* indicates a reference value and ζ is the zeta potential.

- Laplace equation

$$\sigma^* \frac{\partial^2 \phi^*}{\partial x_i^{*2}} = 0 \quad (19)$$

where

$$\sigma^* = \frac{\sigma_p}{\sigma_{ref}}$$

- Poisson-Boltzmann equation

$$\frac{\partial^2 \psi^*}{\partial x_i^{*2}} = -(\kappa L_{ref})^2 \sinh(\psi^*) \quad (20)$$

where κ^{-1} is known as Debye length and corresponds to the EDL characteristic thickness (Patankar and Hu, 1998)

$$\kappa^{-1} = \left(\frac{k_{Bo} T \epsilon \epsilon_0}{2n_0 z^2 e^2} \right)^{1/2}$$

and the reference length, L_{ref} , corresponds to the channel width.

- Continuity equation

$$\frac{1}{\beta^{*2}} \frac{\partial p^*}{\partial t^*} = -\rho^* \frac{\partial \bar{u}_i^*}{\partial x_i^*} \quad (21)$$

where the artificial compressibility parameter, β , (Nithiarasu, 2003) is locally calculated at each node as (Massarotti et al., 2006):

$$\beta = \max(\eta, u_{conv}, u_{diff}) \quad (22)$$

The constant η is assumed to be 0.5, u_{conv} and u_{diff} are the convective and diffusive velocities, respectively.

- Momentum equation

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$$\frac{\rho^*}{\Phi} \left(\frac{\partial \bar{u}_i^*}{\partial t^*} + \frac{1}{\Phi} \frac{\partial (\bar{u}_i^* \bar{u}_j^*)}{\partial x_j^*} \right) = -\frac{\partial p^*}{\partial x_i^*} + \frac{1}{\Phi Re} \frac{\partial^2 \bar{u}_i^*}{\partial x_i^{*2}} - \frac{1}{Re Da} \bar{u}_i^* - \frac{c_F}{Da^{1/2}} |\mathbf{V}| \bar{u}_i^* + \Phi (J \sinh(\psi^*) + J_{eff}) \left(-\frac{\partial \phi^*}{\partial x_i^*} \right) \quad (23)$$

where

$$Re = \frac{\rho_{ref} u_{ref} L_{ref}}{\mu_f} = \rho_{ref} \left(\frac{E_x \epsilon \epsilon_0 \zeta}{\mu_f} \right) \left(\frac{L_{ref}}{\mu_f} \right) \quad Da = \frac{K}{L_{ref}^2};$$

$$J = \frac{2n_0 k_{Bo} T}{u_{ref}^2 \rho_{ref}} \quad J_{eff} = \frac{\Phi \epsilon \epsilon_0 \zeta_p}{K} \frac{k_{Bo} T}{z e u_{ref}^2 \rho_{ref}} \left(\frac{2I_1(\kappa R_{pore})}{\kappa R_{pore} I_0(\kappa R_{pore})} - 1 \right) \quad (24)$$

From here onwards the volume averaged components of velocity will be indicated as u_i instead of \bar{u}_i , for the sake of simplicity.

The above set of non-dimensional equations has been solved by using fully explicit artificial compressibility-based CBS scheme (Nithiarasu, 2003; Nithiarasu et al., 2016).

2.1.2 Boundary and Initial Conditions

The layout of the micro-channel considered in this work is shown in Figure 2, with the boundary conditions applied.

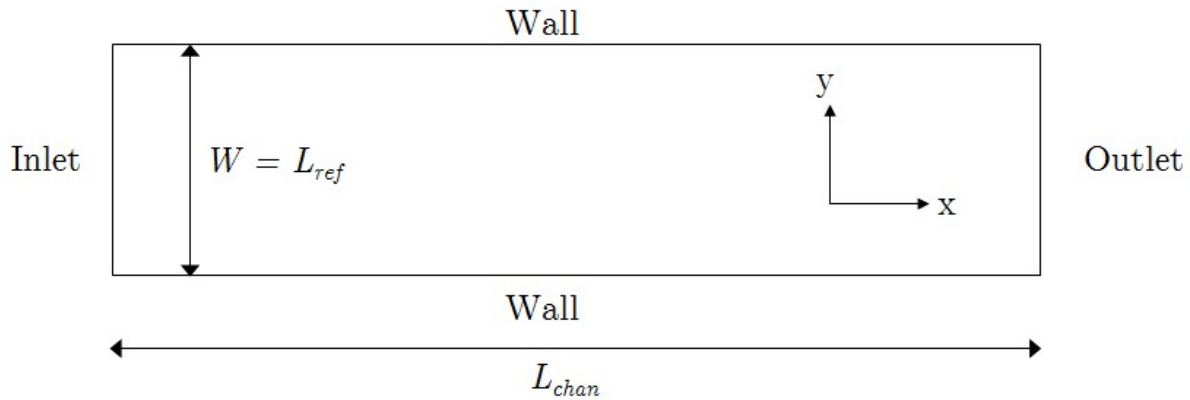


Figure 2: Rectangular 2D micro-channel considered in the simulations.

An external potential difference between the inlet and outlet, $\phi_1^* - \phi_2^*$, is considered to be applied, and the normal components of velocity gradients are assumed to be zero at both inlet and outlet.

$$\begin{aligned} \text{at } : x = 0 \quad & \frac{\partial \psi^*}{\partial x^*} = 0; \quad \phi^* = \phi_1^*; \quad \frac{\partial u_i^*}{\partial x^*} = 0; \\ \text{at } : x = L_{chan} \quad & \frac{\partial \psi^*}{\partial x^*} = 0; \quad \phi^* = \phi_2^*; \quad \frac{\partial u_i^*}{\partial x^*} = 0; \end{aligned} \quad (25)$$

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The channel walls are assumed to be active with a prescribed non-dimensional modified zeta potential, ζ'_w , and to obey no-slip velocity boundary conditions; the external potential gradient in y direction is equal to zero:

$$\psi^* = \zeta'_w; \quad \frac{\partial \phi^*}{\partial y^*} = 0; \quad u_1^* = 0 \quad (26)$$

ζ'_w is considered to take into account the effect of charged solid particles on internal potential distribution within the micro-channel (Tang et al., 2010) and the possible overlap between the internal potential of particles and channel walls (Scales and Tait, 2006). Considering the linearized Poisson-Boltzmann equation, the model proposed by Rice and Whitehead (1965) is used to define the modified wall zeta potential (Rice and Whitehead, 1965) as:

$$\zeta'_w = \zeta_p \left(1 - \frac{2I_1(\kappa R_{pore})}{\kappa R_{pore} I_0(\kappa R_{pore})} \right) + \zeta_w - \zeta_p \quad (27)$$

where ζ_p is the zeta potential of the porous material.

The computation is started with prescribed zero velocity components as the initial condition.

3 Results and discussions

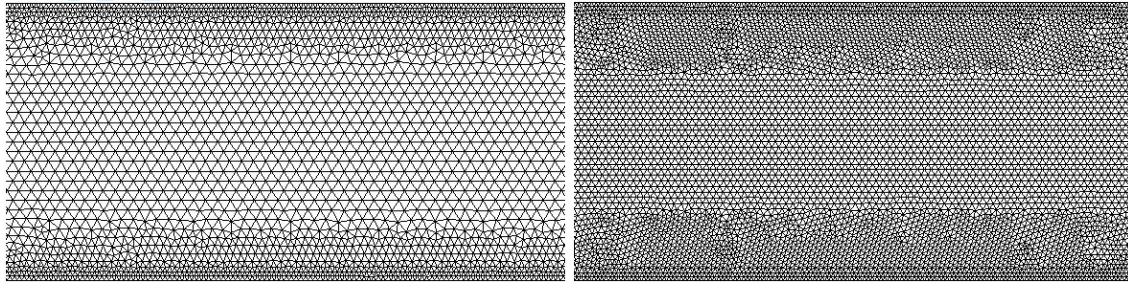
The proposed numerical model is used to investigate EO in free channels and channels packed with porous media, in order to assess the effectiveness of using porous media to enhance EOF.

A silicon micro-channel of $30 \mu m$ in width, characterized by an aspect ratio of 10, with deionized water as working fluid is considered as a reference case study. The electrical conductivity, σ_p , and dynamic viscosity, μ_f , are assumed to be constant. The zeta potential acting on channel walls and, in case of EOF through porous media, on the boundaries of the solid particles, is assumed to be equal to $-19 mV$. This value corresponds to a modified zeta potential equal to $-15 mV$ (see Equation 27). The value considered for the zeta potential imposed on the charged surfaces is derived from some experimental investigations carried out on electro-osmotic flow in silicon microchannels (Eng and Nithiarasu, 2009). An external electric field of $1 kV/m$ is applied. The other parameters used in this study are reported in Table 1.

Table 1: Parameters used in the numerical simulations.

Parameter	Measurement unit	Value
Dielectric constant of the electrolyte, ϵ	78.4	-
Permittivity of vacuum, ϵ_0	$8.85 \cdot 10^{-12}$	$C \cdot (V \cdot m)^{-1}$
Ionic concentration in the bulk solution, n_0	$6.022 \cdot 10^{19}$	m^{-3}
Valence of the ions, z	1	-
Elementary charge, e	$1.602 \cdot 10^{-19}$	C
Boltzmann constant, k_B	$1.381 \cdot 10^{-23}$	$m^2 kg \cdot (s^2 K)^{-1}$
Temperature, T	298	K
Fluid density, ρ	1000	$kg \cdot m^{-3}$
Fluid viscosity, μ	$8.91 \cdot 10^{-4}$	$Pa \cdot s$

265 In channels packed with porous media, a porosity equal to 0.8 is assumed. The porous medium is composed
 266 of silicon circular particles with a diameter equal to 16% of the channel width.
 267 A set of 2D unstructured meshes, refined near all the solid boundaries to capture the rapid change in both
 268 internal potential and velocity, is used. The details of the meshes used for plain channels and channels with
 269 obstructions are shown in Figure 3. A mesh sensitivity study has been carried out to finalise the meshes used
 270 in the calculations.



(a) Free channel.

(b) Porous medium channel.

Figure 3: Meshes of micro-channels considered in the simulations.

3.1 Verification of the model

272 The numerical model described in Section 2 is used to determine EOF in free channels and channels packed
 273 with porous media. The results are compared to the available analytical solutions.

274 For a two dimensional rectangular channel, the analytical solution for the internal potential in free channels
 275 can be written as (Patankar and Hu, 1998):

$$\psi = \frac{\cosh[\kappa W (y - 1/2)]}{\cosh[\kappa W / 2]} \quad (28)$$

276 where y is the distance from the wall and W is the channel width. The analytical solution for the horizontal
 277 velocity component in free channels (Arnold, 2007) may be expressed as:

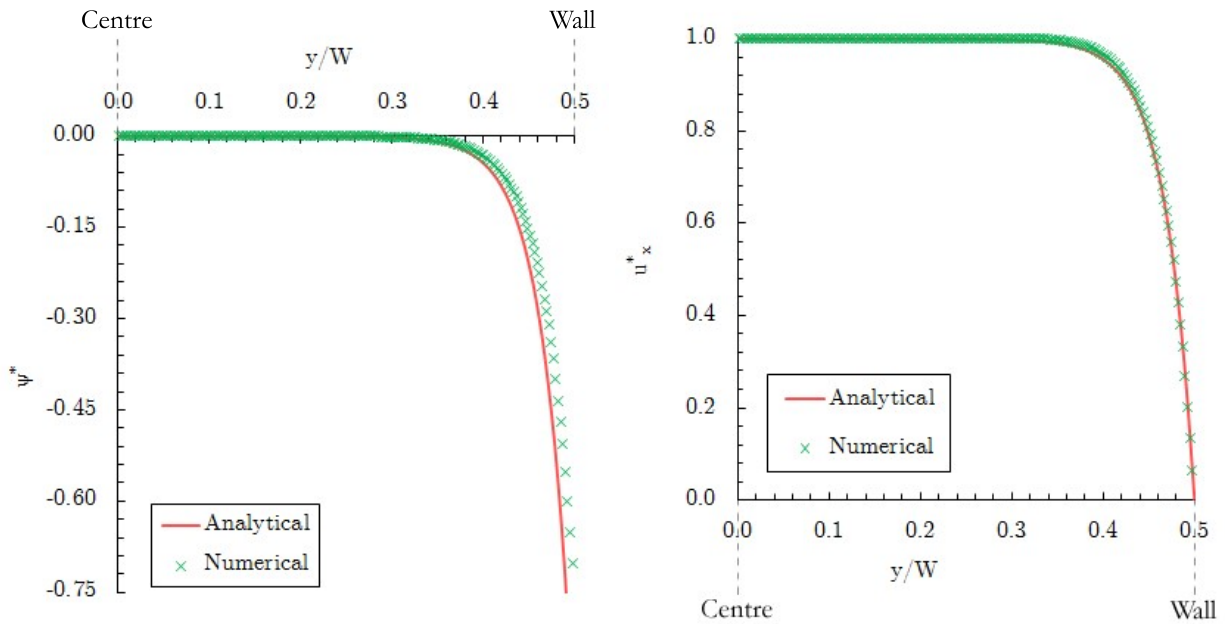
$$u = 1 - \zeta \left(2 \ln \frac{1 + \exp(-\kappa W y) \tanh(\frac{1}{4} \zeta_w)}{1 - \exp(-\kappa W y) \tanh(\frac{1}{4} \zeta_w)} \right) \quad (29)$$

278 In Figure 4, the internal potential and velocity profiles in free channels are plotted. In all plots, the quantities
 279 are non-dimensional, and half width of the channel is considered for the sake of clarity.

280 Since the analytical solution is derived for the linearized Poisson-Boltzmann equation, there is a slight
 281 discrepancy between the analytical solution and the numerical results. The data of the simulations for
 282 velocity are normalised against the maximum velocity in order to have a clear comparison with the analytical
 283 solution.

284 For EOF in channels packed with porous media, Scales and Tait proposed different analytical solutions
 285 (Scales and Tait, 2006). For EOF between two parallel plates in a porous channel of width W , with a

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(a) Internal potential profile.

(b) Horizontal velocity profile.

Figure 4: Comparison of the present results with analytical solutions in free channels for the reference case study. Half width of the channel is plotted for the sake of clarity.

modified zeta potential ζ'_w applied at the channel walls, the solution to the linearized Poisson-Boltzmann equation can be expressed as:

$$\psi(y) = \left(\zeta'_w \frac{\sinh(\sqrt{\tau}\kappa y)}{\sinh(\sqrt{\tau}\kappa W)} + \zeta'_w \frac{\sinh(\sqrt{\tau}\kappa(c-y))}{\sinh(\sqrt{\tau}\kappa W)} \right) \quad (30)$$

In the analysed case, the tortuosity, τ is assumed to be equal to 1. For the horizontal velocity two different cases can be analysed:

- uncharged walls and charged porous medium ($\zeta_w = 0$)

$$\bar{u}(y) = \bar{u}_d \left(1 - \frac{e^{-\lambda(W-y)} - e^{-\lambda(2W-y)} + (1 - e^{-\lambda W}) e^{-\lambda y}}{1 - e^{-\lambda 2W}} \right) \quad (31)$$

where \bar{u}_d is given by the Darcy's law, as

$$\bar{u}_d = -\frac{K}{\sqrt{\tau}\mu_{eff}} (\nabla p + \rho_{eff}\nabla\phi) \quad (32)$$

and λ is the Brinkmann screening length defined as

$$\lambda = \sqrt{\frac{\Phi\sqrt{\tau}\mu_{eff}}{K\mu_f}} \quad (33)$$

- 293 • charged walls and uncharged porous medium ($\zeta_p = 0$)

$$\bar{u}(y) = Z \left(\frac{\psi_{w1} (e^{-\lambda(2W-y)} - e^{-\lambda y}) + \psi_{w2} (e^{-\lambda(W+y)} - e^{-\lambda(W-y)})}{1 - e^{-\lambda 2W}} \right) \quad (34)$$

$$+ Z\psi(y) = Zu_B(y) + Z\psi(y)$$

$$Z = \frac{\epsilon\epsilon_0\kappa^2\nabla\phi}{\mu_f(\lambda^2 - \tau\kappa^2)} \quad (35)$$

295 The superposition of the individual cases, Eq.s (31) and (34), is used to analyse the case of charged walls
296 and charged porous medium.

297 In Figure 5, the profiles of internal potential and velocity, in the case of EOF through porous media, are
298 plotted and compared to their analytical solution. A good agreement between the results of the proposed
299 algorithm and the analytical solutions is found. The internal potential profile is similar in shape to that
300 obtained for free channels (see Figure 4a), but different in magnitude since the modified zeta potential is
301 applied on channel walls. A slight increase of the horizontal velocity can be observed in the region close to
the channel walls. The analytical solutions proposed by Scales and Tait (2006) are also used to determine

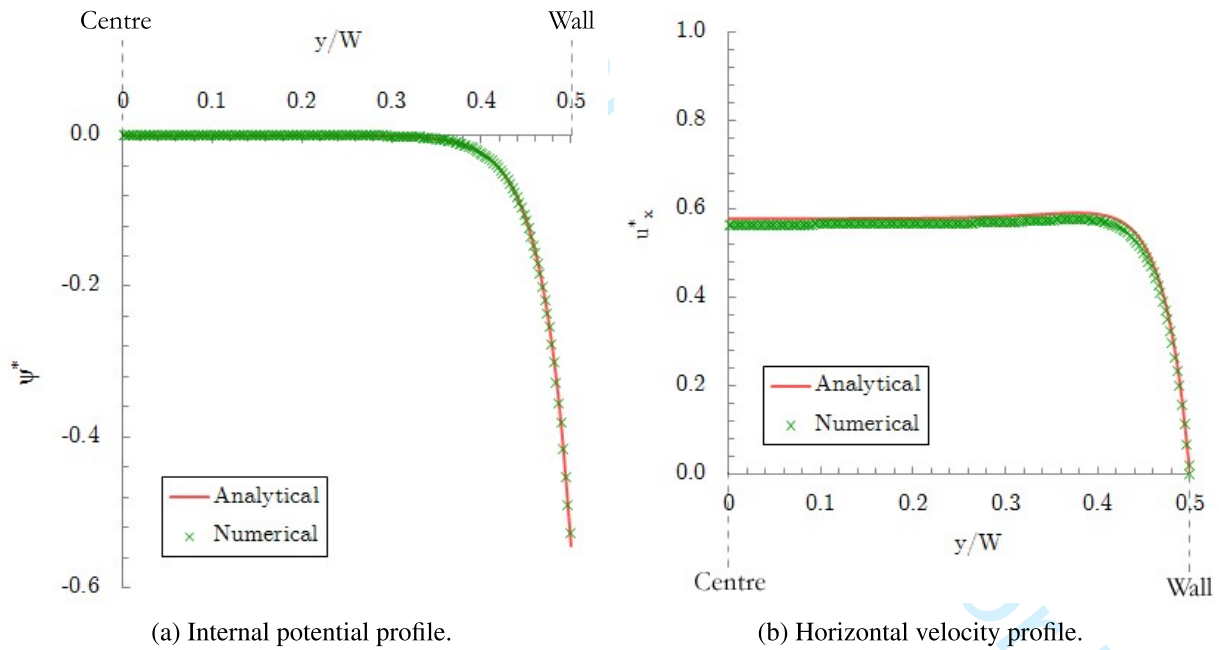
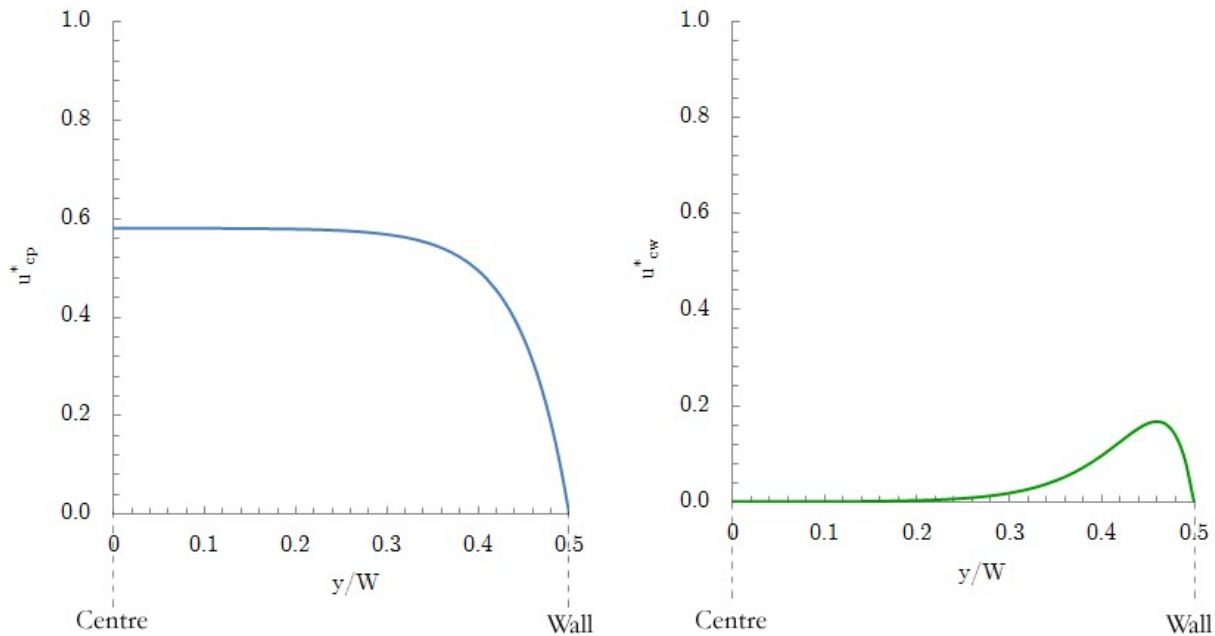


Figure 5: Comparison of results from numerical simulations against analytical solutions in channels packed with porous media for the reference case study. Half width of the channel is plotted for the sake of clarity.

302
303 EO velocity in case of charged particles with neutral walls, u_{cp}^* , (Figure 6a), and for charged walls with
304 neutral particles, u_{cw}^* , (Figure 6b), in order to assess the influence of charged particles and of charged walls
305 on EOF. The average velocity is significantly higher in the case of charged particles and neutral walls, u_{cp}^* ,
306 than in the case of charged walls and neutral particles, u_{cw}^* .

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(a) Charged particles and neutral walls.

(b) Charged walls and neutral particles.

Figure 6: Horizontal velocity profile. Half width of the channel is plotted for the sake of clarity.

Two important conclusions can be drawn from this analysis:

- solid charged particles have a strong influence on EOF driven systems;
- neglecting the effect of charged media in micro-channels on EOF, as done in many previous works concerning EOF through porous media, can have a strong influence on the solution of the model.

3.2 Sensitivity analyses

The effect of several parameters on EOF through porous media is investigated in order to find optimal values for the flow. To this aim, the parameters governing electro-kinetic phenomena responsible for fluid flow are analysed through the algorithm for EOF based on the generalized model for porous media flow.

3.2.1 Effect of micro-channel width on EOF

The geometry of the micro-channel significantly influences EOF. For this reason, this parameter is investigated, comparing its effect in free channels and channels packed with porous media. A range of different channel widths, W , between $5\mu\text{m}$ and $150\mu\text{m}$, is considered. The profiles of internal potential and horizontal velocity at the outlet section of the channel are reported for different channel widths in Figures 7 and 8, respectively.

In both cases, as the channel width increases, the internal potential presents higher gradients close to the

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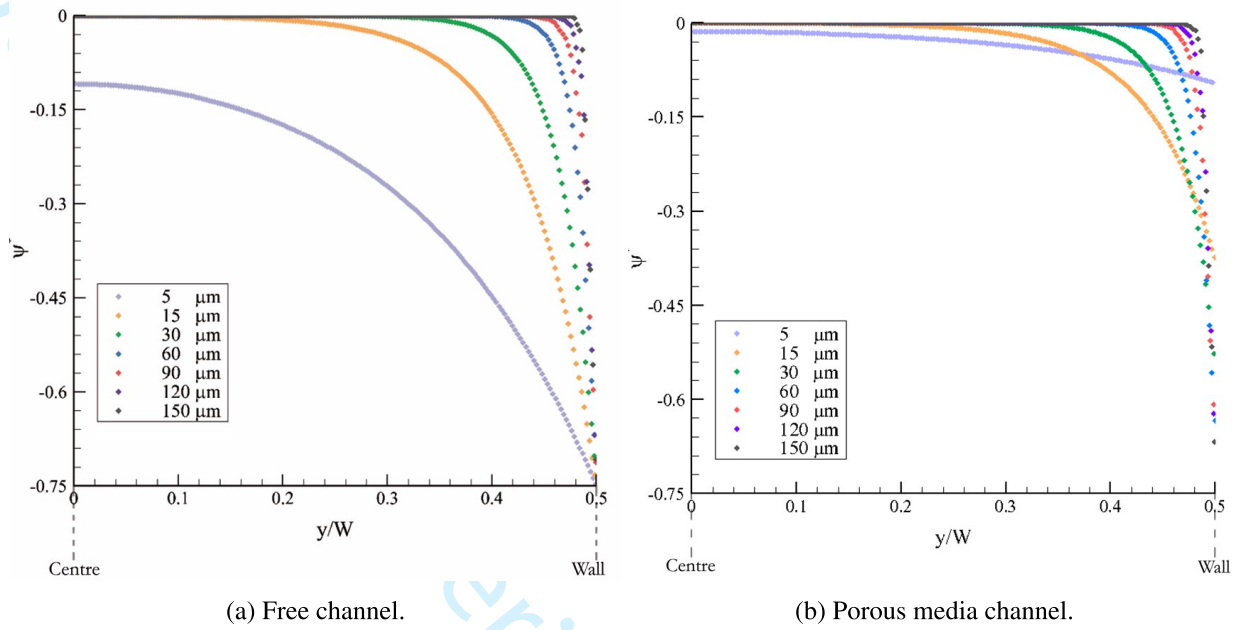


Figure 7: Internal potential at different channel widths.

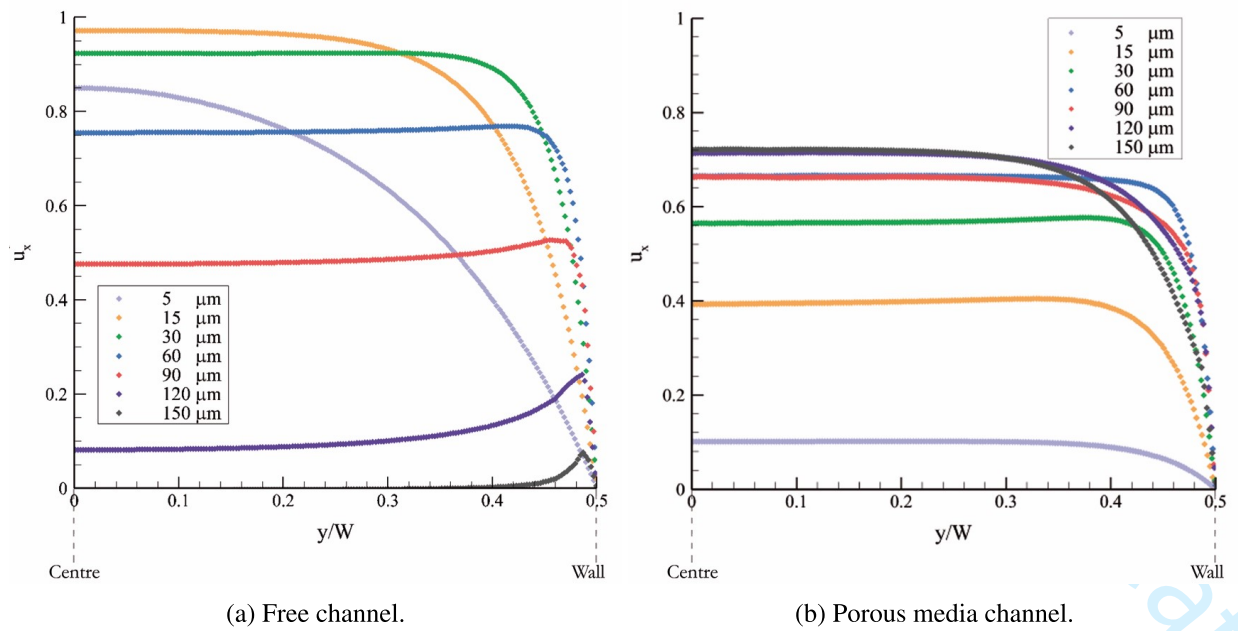


Figure 8: Horizontal velocity at different channel widths.

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channel walls and goes to zero in the central region of the channel. This behaviour is weaker in porous media channels, where the charge of the particles balances the increase of width effect. In the case of free channel the zeta potential applied on the channel walls does not vary with the channel width. In channels packed with porous media, the zeta potential, imposed as a boundary condition on the channel walls for internal potential, varies with porosity and particle size. In the current analysis the porosity is constant and assumed equal to 0.8, whereas the particle diameter varies with the channel width. As the channel width increases, the particle diameter increases and then the magnitude of the zeta potential and the maximum internal potential increase. However, the modified zeta potential, used in the case of porous media channel, is always lower than the zeta potential really acting on channel walls and used for the simulation of the free channels. For the sake of clarity, the values of modified zeta potential at different channel widths are reported in Table 2. It is important to remember that the zeta potential acting on the channel walls is equal to -19 mV.

Table 2: Modified zeta potential, ζ'_w , calculated for different values of channel width.

Channel width W μm	Modified zeta potential ζ'_w mV
5	-2.45
15	-9.63
30	-13.9
60	-16.5
90	-17.4
120	-17.8
150	-18.1

The internal potential significantly influences EO velocity. In the free channel, the average velocity increases with the channel width in a very small range of micro-channel widths, from 5 to 15 μm , while beyond this value it rapidly decreases (See Figure 8a). This is due to the increase in the distance between the channel walls that lowers the effect of the EDL potential, reducing the average velocity. For this reason, EO flow in free channel is applied only at micro scale. As shown in Figure 8b, in porous media channels the average velocity rapidly increases in the same range of channel width (from 5 to 15 μm), but it is lower than in free channels. This is due to the modest value of zeta potential applied on the channel walls, and to the small distance between particles, that causes higher resistance to fluid flow. The higher the channel width, the higher the average velocity. Beyond 60 μm , the velocity is higher than in free channels. Moreover, beyond this value the influence of the charge of channel walls decreases and EOF is mainly due to the charge of solid particles. In fact, the velocity profile approaches that observed in the case of charged particles and uncharged walls (See Figure 6a). As the channel width further increases, the variability of average velocity with channel width tends to decrease.

The results in terms of flow rate are reported in Table 3, together with the results obtained for the free channel.

Table 3: Flow rate for different micro-channel widths with and without porous media.

Channel width μm	Flow rate in micro-channel packed with porous media $\mu m^2 min^{-1}$	Flow rate in free channel $\mu m^2 min^{-1}$
5	$3.63 \cdot 10^{-4}$	$2.87 \cdot 10^{-3}$
15	$4.57 \cdot 10^{-3}$	$1.18 \cdot 10^{-2}$
30	$1.48 \cdot 10^{-2}$	$2.41 \cdot 10^{-2}$
60	$3.26 \cdot 10^{-2}$	$4.10 \cdot 10^{-2}$
90	$4.84 \cdot 10^{-2}$	$4.01 \cdot 10^{-2}$
120	$5.91 \cdot 10^{-2}$	$1.21 \cdot 10^{-2}$
150	$6.31 \cdot 10^{-2}$	$2.32 \cdot 10^{-4}$
180	$1.09 \cdot 10^{-1}$	-
210	$1.28 \cdot 10^{-1}$	-
240	$1.47 \cdot 10^{-1}$	-

The analysis confirms the efficacy of EO to drive flow through porous media. It is worth to notice that, contrary to what happens in free channels, the flow rate through porous media increases in the whole range of channel widths analysed. As mentioned above, for larger channel widths, EO is mainly affected by the charge of solid particles, rather than that of channel walls. For this reason, EO can be effectively used to drive flow through porous media independently on the scale of the system, contrary to what happens in free fluid systems, where the efficiency of EO as driving force becomes negligible as the scale of the system increases.

3.2.2 Effect of solid particle diameters on EOF

Several parameters depend on the diameter of solid particles. It affects the hydraulic radius, Eq. (16), and, as a consequence, the modified zeta potential applied on the channel walls, Eq. (27), and the non dimensional parameter that takes into account the effect of charged solid particles on EOF, Eq. (24). Moreover, the solid particle diameter influences the permeability of the porous medium, Eq. (13), and, therefore, the fluid velocity. The reference case (P16% from now on) is simulated by varying the diameter of solid particles, that is here assumed equal to 12% (P12% from now on) and 29% (P29% from now on) of the channel width, by keeping constant the porosity. The horizontal velocity profiles for the particle sizes considered are shown in Figure 9.

The average velocity is higher when the porous medium is made of larger particles, with a higher difference at smaller channel widths. In the range between 5 and $30\mu m$, also the rate of increase of the average velocity is higher in P29% than in P16%. These trends appear to be affected by the modified zeta potential, applied as a boundary condition on channel walls, and the permeability. As shown in Fig. 10, the higher the particle size, the higher the zeta potential in absolute value and the permeability of the porous medium.

This could explain the higher velocities found for larger particles. Smaller the channel width, smaller the

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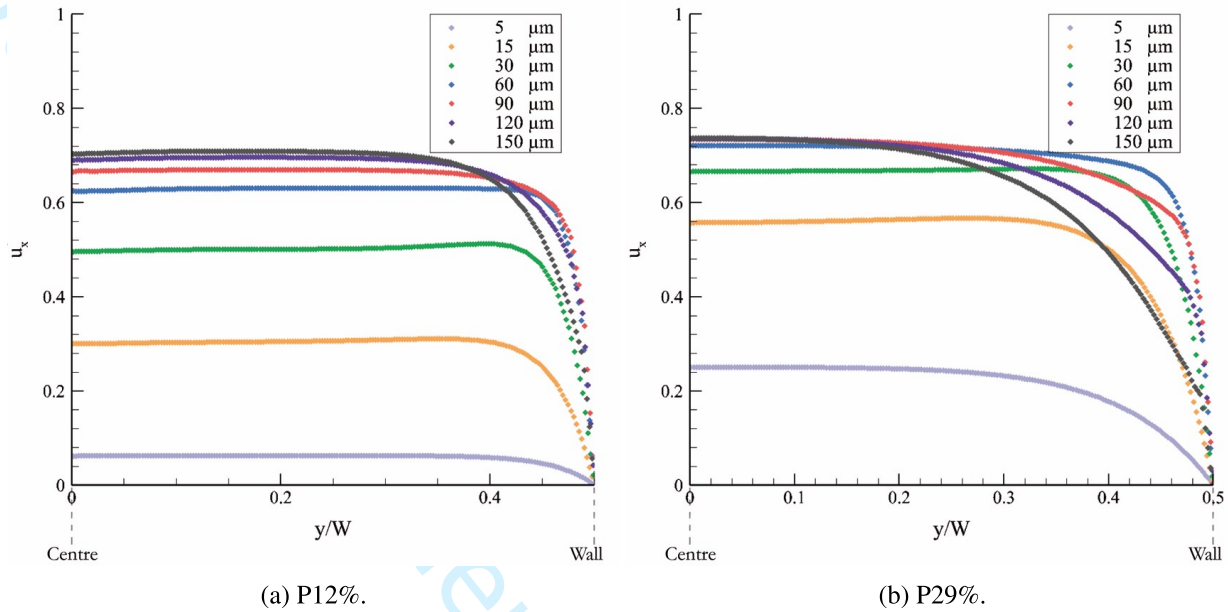


Figure 9: EO velocity at different particles sizes plotted at different channel widths.

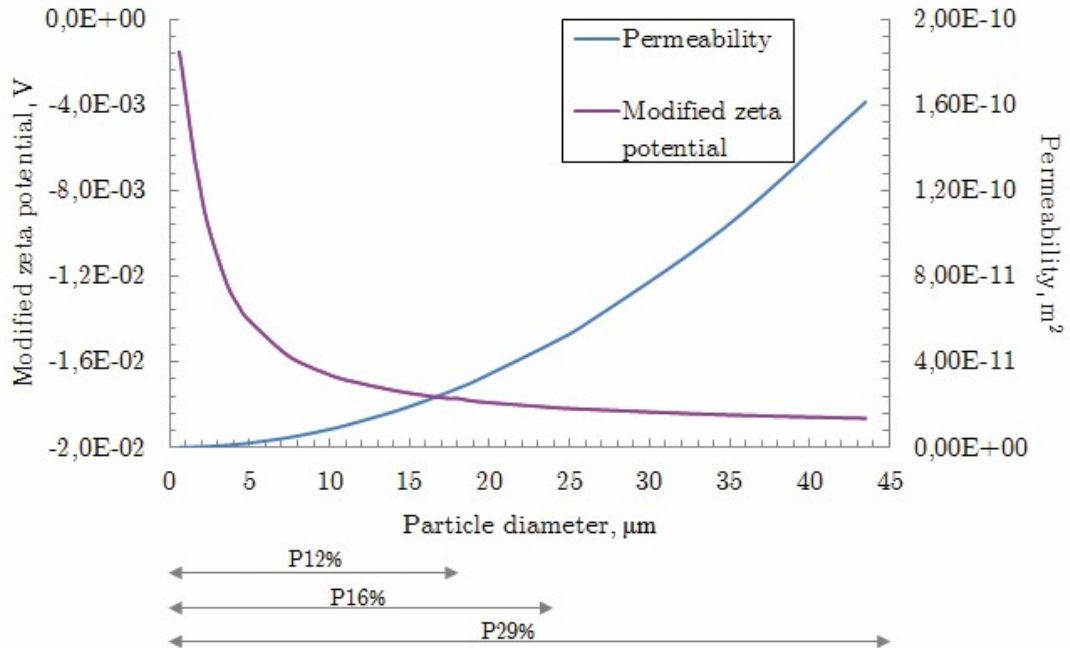


Figure 10: Variability of modified zeta potential and permeability with particle diameter. The range of the three cases analysed, P12%, P16% and P29%, is shown for the sake of clarity.

particle size: in the lower range of channel widths, the higher difference between the two cases can be explained considering the fast growth in absolute value of the modified zeta potential. The use of larger particles reduces the increase of velocity near the walls; in both cases it further decreases as the channel width is larger than $90\mu m$. Beyond this value, the velocity profile tends to that obtained in case of charged particles and uncharged walls (See Figure6a), indicating a strong influence of the charge of solid particles. At the upper bound of the range considered for the channel width, the difference in maximum velocity decreases for the two cases analysed. This aspect is more evident in Fig. 11, where all of the particle sizes analysed are compared in terms of flow rate.

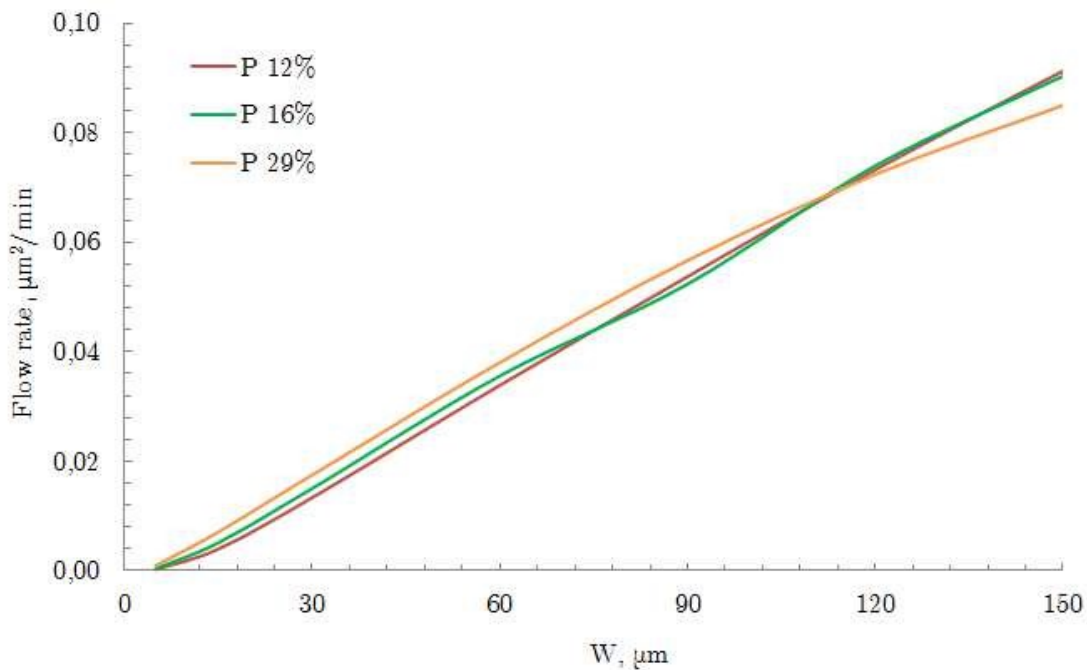


Figure 11: Flow rate at different widths of micro-channels with varying particle diameter.

In the case of smaller particles (P12%), the trend is very similar to that of the reference case (P16%). It is worth noticing that, the flow rate grows with particle size, up to a channel width equal to roughly $110\mu m$, whereas beyond this value the use of larger particles produces lower flow rate, even though their use enhances permeability. In this last case, the flow rate even decreases as the channel width exceeds $120\mu m$. This can be explained by considering the internal potential and horizontal velocity distributions within the channel, illustrated in Fig. 12. The thickness of EDL is the same for both the particles sizes analysed at the same channel width, as shown in Figures 12a and 12b, 12c and 12d. The difference is in the magnitude of internal potential: as mentioned above, a higher zeta potential in absolute value is imposed in case of larger particles and this increases the internal potential near the walls. As shown in Figure 10, such an increase is considerable up to a particle size of $10\mu m$, whereas beyond this value the trend is approximately constant. For this reason, the distributions shown in Figures 12c and 12d, corresponding to a particle diameter equal to $14\mu m$ and $35\mu m$, respectively, are similar. In terms of velocity, the difference between the cases taken into account is more significant. In channels of $30\mu m$ in width, a substantial decrease in velocity can be

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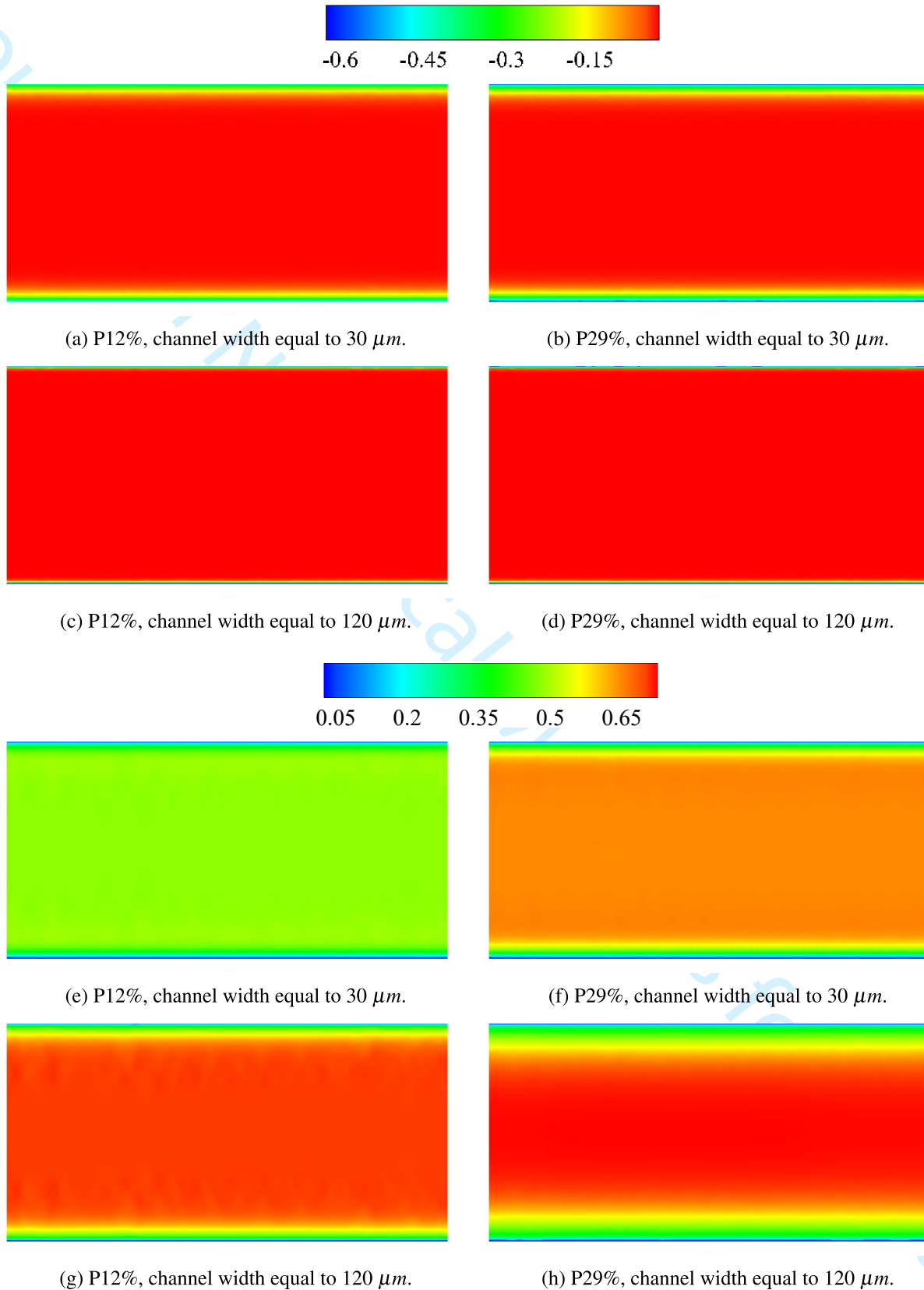


Figure 12: Internal potential (a-d) and horizontal velocity (e-h) distributions.

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observed with smaller particles, whereas at $120 \mu m$ the difference between the two cases is reduced. At this channel width the maximum velocity is higher in the case of larger particles. This divergence can be attributed to the difference in permeability, that can be appreciated in Figure 10 by considering a particles diameter equal to 14 and $35 \mu m$.

3.2.3 Effect of zeta potential on EOF

The zeta potential characterizing channel walls and solid particles significantly affects the internal potential distribution and, as a consequence, EOF. It should be noticed that in case of channels packed with porous media, a modified zeta potential is applied as a boundary condition to the channel walls. Its values, when channel walls and solid particles have the same zeta potential, are reported in Table 4.

Table 4: Modified zeta potential, ζ'_w , calculated for different values of zeta potential acting on channel walls, ζ_w , and solid particles, ζ_p .

$\zeta_w = \zeta_p$ mV	ζ'_w mV
-5.00	-3.61
-10.00	-7.23
-19.00	-13.73
-30.00	-21.69
-50.00	-36.14
-75.00	-54.22

In Figure 13, the velocity profile is shown for free channels at several values of the walls zeta potential, and for channels packed with porous media at several values of walls and particles zeta potential.

The influence of the zeta potential on EO velocity is very low in the free channel and essentially null in channels packed with porous media. A different outcome is obtained when the zeta potential of walls, ζ_w and that of the particles ζ_p , are assumed to be different from each other. The modified zeta potential imposed on channel walls depend on both ζ_w and ζ_p . Its values for the two cases analysed are reported in Tables 5 (a) and (b).

First, a constant value of ζ_w is considered, whereas ζ_p is varied, as shown in Figure 14a. In this case, as ζ_p increases in absolute value, velocity increases. By keeping constant ζ_p and varying ζ_w , as illustrated in Figure 14b, EOF reduces as the difference between ζ_p and ζ_w increases, and, as expected, the velocity near the walls grows when ζ_w is much higher than ζ_p . This trend agrees with the results observed by Liapis and Grimes (2000), discussed in Section 1.

It is worth noticing that EO average velocity tends to decrease and to become constant as the zeta potential of solid particles increases and that of channel walls decreases. The velocity drops faster in case of variable

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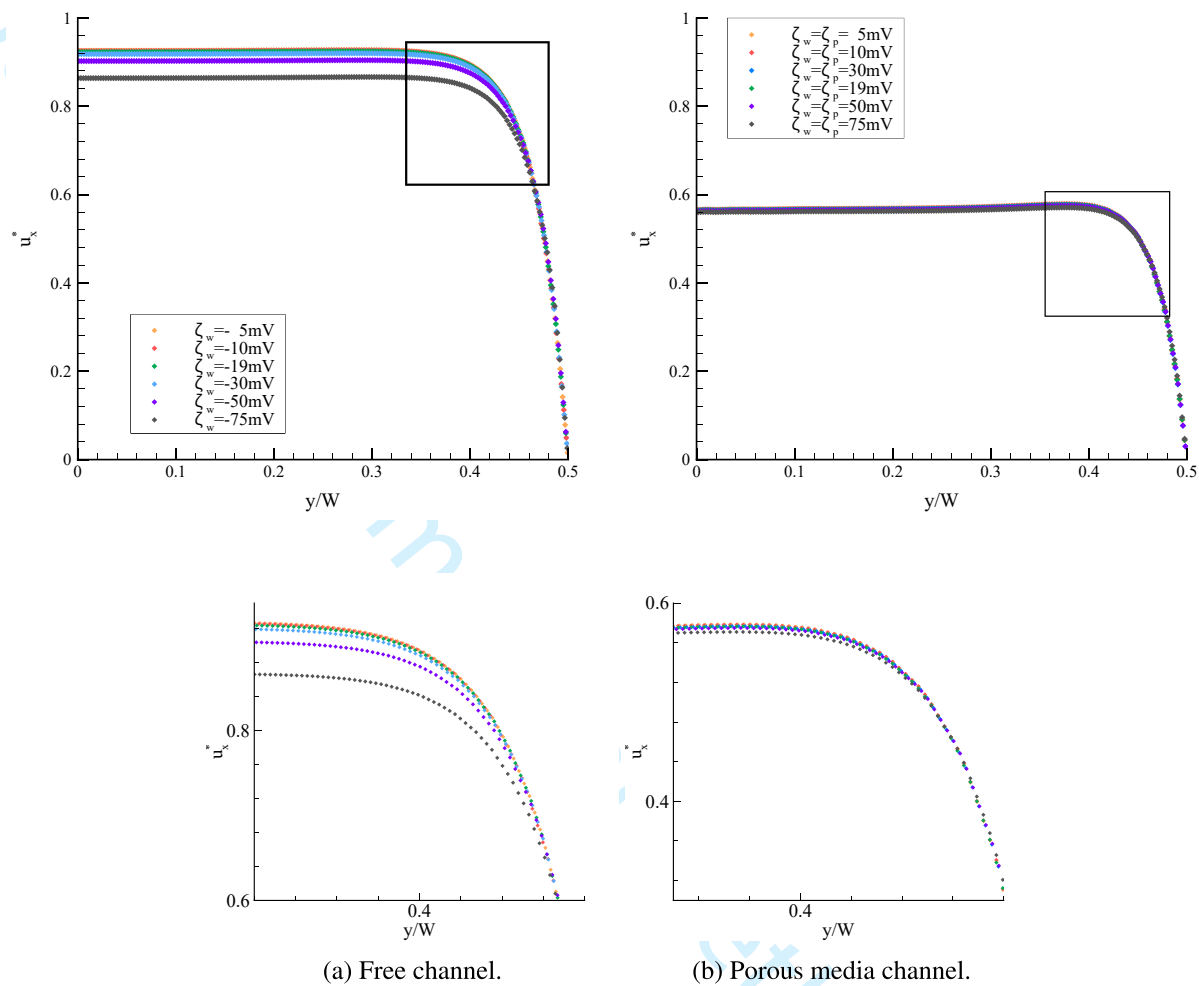


Figure 13: EO velocity at different values of zeta potential, considering the same quantity for channel walls and solid particles.

Table 5: Modified zeta potential, ζ'_w , calculated for different values of zeta potential acting on channel walls, ζ_w , and solid particles, ζ_p .

(a) $\zeta_w = -19\text{mV}$		(b) $\zeta_p = -19\text{mV}$	
ζ_p mV	ζ'_w mV	ζ_w mV	ζ'_w mV
-5	-17.61	-5	0.6
-10	-16.23	-10	-4.23
-19	-13.73	-19	-13.73
-30	-10.69	-30	-24.73
-50	-5.14	-50	-44.73
-75	1.78	-75	-69.73

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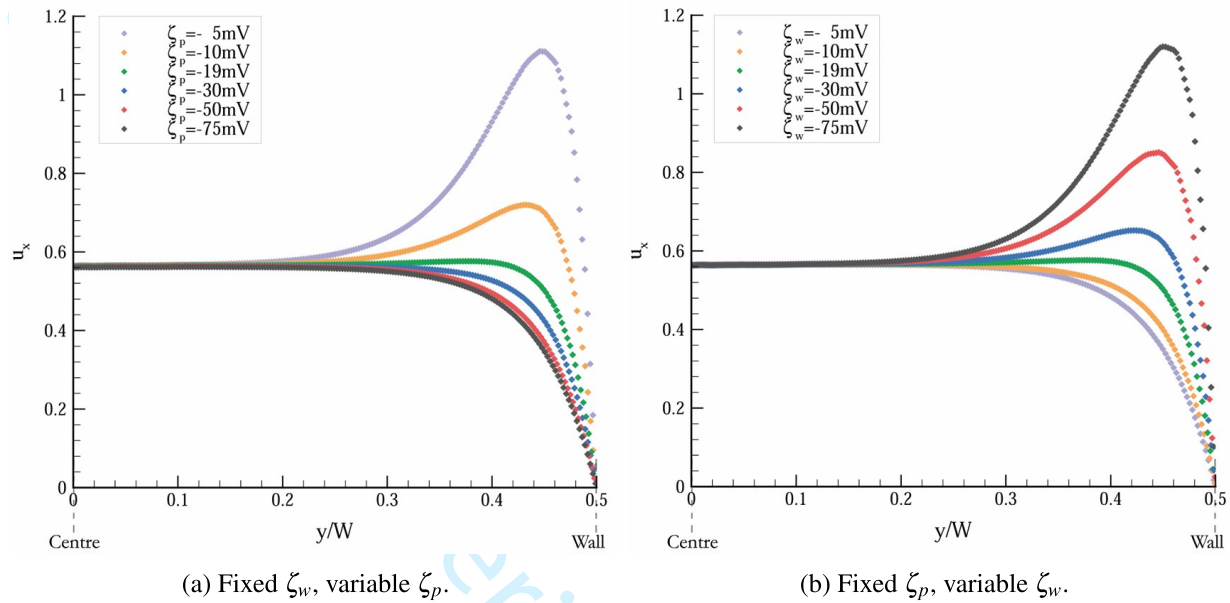


Figure 14: Velocity at different values of zeta potential of solid particles and channel walls.

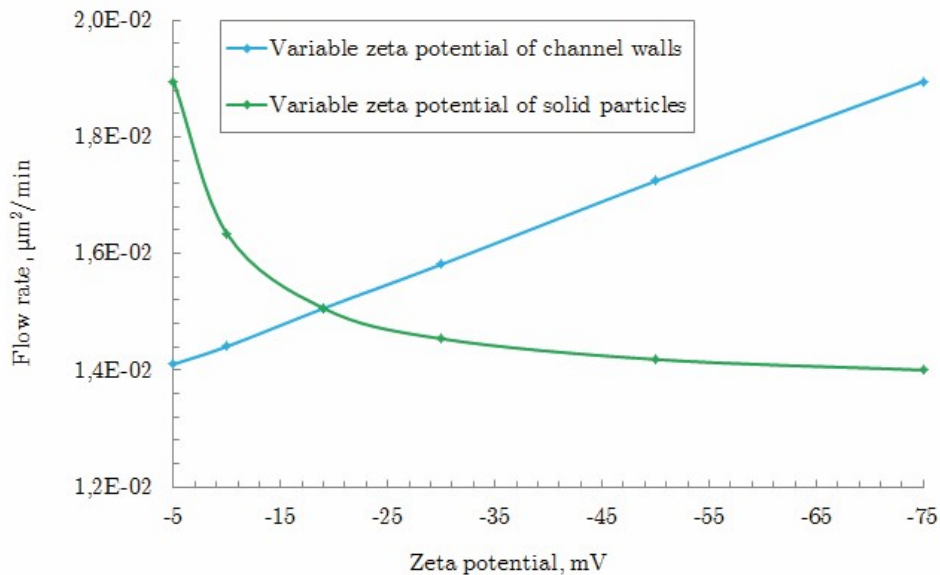


Figure 15: Flow rate at different values of modified zeta potential, with varying zeta potential of channel walls and solid particles.

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ζ_w , as confirmed by the plot in Figure 15. Flow rate rapidly decreases as ζ_p increases in absolute value up to -30 mV, then it becomes approximately constant. For fixed ζ_p , the flow rate linearly increases with ζ_w .

3.2.4 Effect of bulk ionic concentration on EOF

The bulk ionic concentration influences the thickness of EDL or Debye length, κ^{-1} . As seen before, this parameter strongly affects EOF. For this reason, in many studies the dependence between the electro-kinetic radius, κW , and EOF has been analysed. Its effect on the velocity is assessed in free channels and channels packed with porous media.

In the analysis of EOF through porous media also the parameter κR_{pore} is taken into account, where R_{pore} is the hydraulic radius, defined in Eq. (16). This quantity affects the modified zeta potential, ζ'_w , imposed on the channels walls.

The variation of both κW and κR_{pore} , and of ζ'_w , with bulk ionic concentration is reported in Table 6.

Table 6: Values of electro-kinetic radius, electro-kinetic hydraulic radius, and modified zeta potential, for different bulk ionic concentrations.

Bulk ionic concentration	Electro-kinetic radius	Electro-kinetic hydraulic radius	Modified zeta potential
n_0 M	κW	κR_{pore}	ζ'_w mV
$0.5E - 05$	7.06	1.51	-3.89
$1.0E - 05$	9.98	2.13	-6.20
$0.5E - 04$	22.3	4.76	-12.0
$1.0E - 04$	31.6	6.73	-13.9
$0.5E - 03$	70.6	15.1	-16.8
$1.0E - 03$	99.8	21.3	-17.5

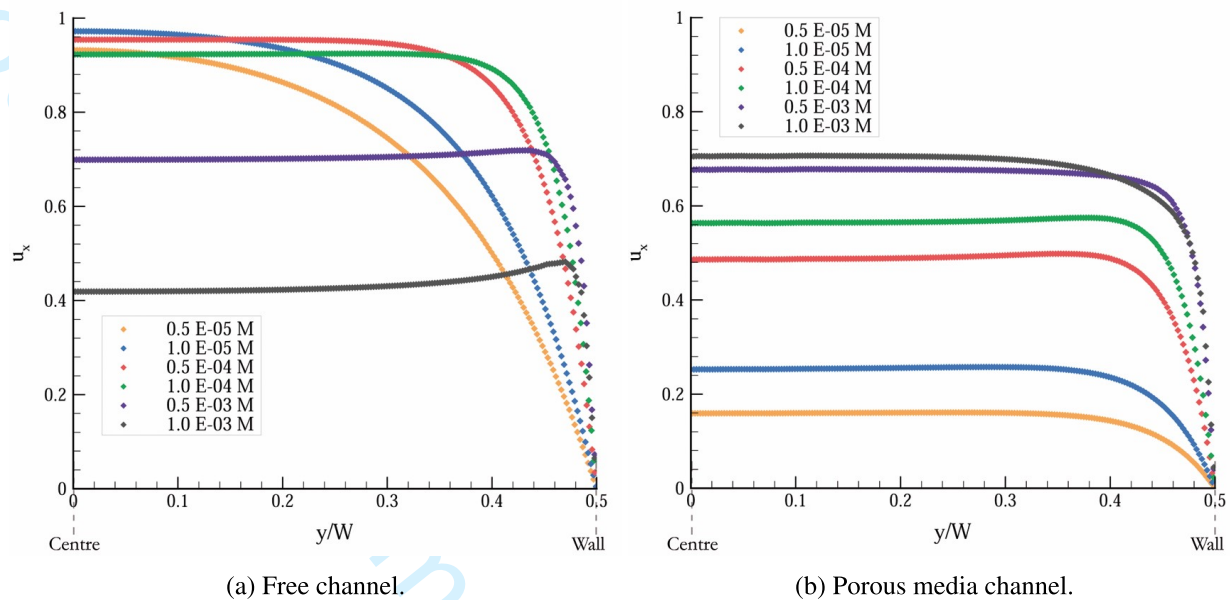
The effect of bulk ionic concentration on horizontal velocity in free channels and channels packed with porous media is shown in Figure 16.

In free channels the average velocity initially increases at increasing bulk ionic concentration, then it starts to decrease. On the contrary, in channels packed with porous media the average velocity increases for increasing bulk ionic concentration in the whole range analysed. As mentioned above, the bulk ionic concentration affects the modified zeta potential, considered in channels packed with porous media. The influence of the zeta potential applied on the channel walls is highlighted in Figure 17, where both the modified zeta potential and the flow rate are plotted against the bulk concentration.

The effect of bulk ionic concentration on EOF can be better understood by analysing the internal potential results illustrated in Figure 18.

At lower concentrations, the EDL thickness is larger and the internal potential is not equal to zero in a larger fraction of the channel, as shown in Figure 18a. Despite this, the maximum absolute value of internal po-

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(a) Free channel. (b) Porous media channel.
 Figure 16: EO velocity at different values of bulk ionic concentration.

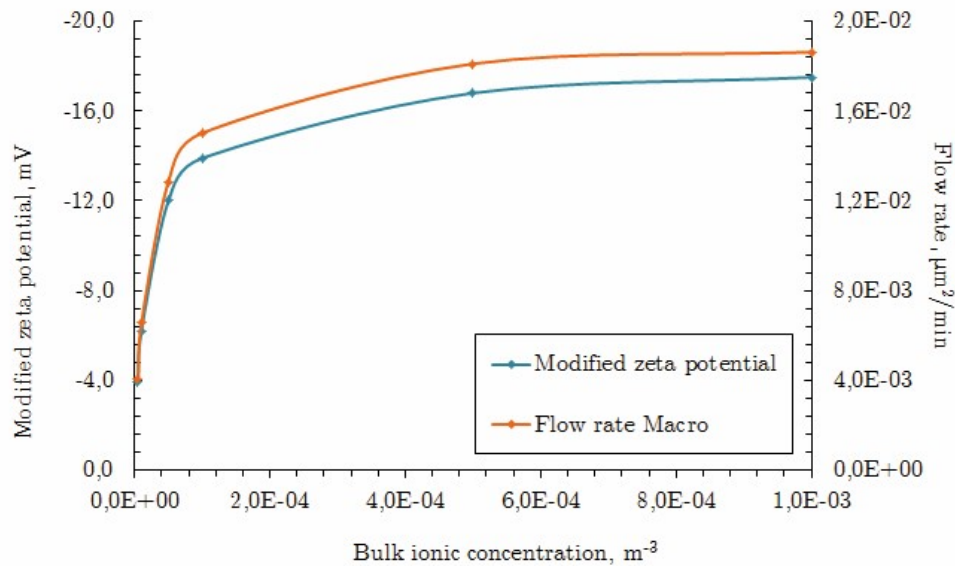


Figure 17: Modified zeta potential and flow rate at different values of bulk ionic concentration.

439 tential, equivalent to the modified zeta potential applied, is lower than that observed at higher concentration
 440 (Figure 18b), and, as a consequence, the average velocity within the channel is lower.

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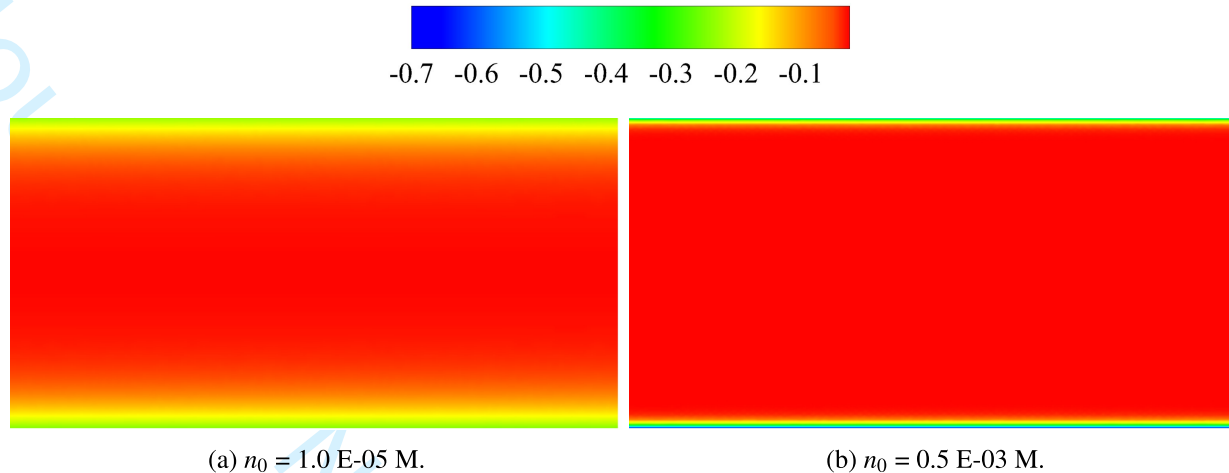


Figure 18: Internal potential in channels packed with porous media at different values of bulk ionic concentration.

4 Conclusions

In this work electro-osmotic flow through porous media is analysed. The porous medium is assumed as a continuum and fluid flow is modelled through the generalized model for porous media flows, modified to take into account the electro-kinetic effects.

The developed model is used to evaluate the effectiveness of using electro-osmosis to drive flow through porous media. The results show that beyond a channel width of $100\mu\text{m}$, the charge of particles composing the porous medium is the main responsible for electro-osmotic flow. This means that electro-osmosis through porous media can be employed independently of the scale of the system, contrary to what occurs in free channels, where electro-osmotic flow decreases as the size of the channel increases. The influence of other parameters is also assessed. The particle size, which affects both the electro-kinetic effect and the flow, is varied to understand its effect on electro-osmotic flow. The electric fluid-solid interaction is taken into account through the zeta potential imposed on the channel walls, used to derive the internal potential distribution. In smaller micro-channels, particle size significantly affects electro-osmotic flow, while at larger channel widths the average velocity appears to be independent of the particle size.

The electric fluid-solid interaction is analysed also by directly considering the variation of zeta potential of both channel walls and solid particles. When these two quantities are identical, the fluid flow does not vary, while if they assume different values, flow can be enhanced. As the difference between the zeta potential of channel walls and that of solid particles increases, the maximum velocity grows. The flow rate increases at higher absolute values of zeta potentials on the channel walls, while it decreases and reaches a constant value when the absolute value of zeta potential of solid particle increases.

Finally, the influence of bulk ionic concentration of the solution on electro-kinetic effect and fluid flow is studied. As this quantity increases, the average velocity presents a rapid initial increase and then becomes approximately constant.

The results obtained from the numerical simulation of electro-osmotic flow in porous media can be used to

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Roman symbol	Unit	Description
b, d	-	Numerical constants
c	$m \cdot s^{-1}$	Speed of sound
c_F	-	Forchheimer coefficient
c_m	<i>Moles</i>	Molar concentration
d_p	m	Particle size
Da		Darcy number
e	C	Elementary charge
E_x	$V \cdot m^{-1}$	External electric field
I		Bessel function
J		Non dimensional parameter
K	$m \cdot s^{-2}$	Permeability
k_{Bo}	$m^2 kg \cdot (s^2 K)^{-1}$	Boltzmann's constant
L	m	Length
n^+		Positive ions
n^-		Negative ions
n_0	m^{-3}	Ionic number concentration
N_A		Avogadro constant
p	$N \cdot m^{-2}$	Pressure
P		Porous term
R_{pore}	m	Average pore size
Re		Reynolds number
T	K	Temperature
u	$m \cdot s^{-1}$	Velocity
\mathbf{V}	$m \cdot s^{-1}$	Velocity vector
W	m	Channel width
z	-	Valence of the ions
Z	-	Non-dimensional parameter

465 define the best geometric and operating conditions for flow enhancement, demonstrating that the proposed
 466 generalised model can be useful as a tool for the optimization of electro-osmotic flow driven systems.

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Acronyms	Description
AC	Alternating Current
CBS	Characteristic Based Split
CEC	Capillary ElectroChromatography
EDL	Electrical Double Layer
EO	Electro-Osmosis
EOF	Electro-Osmotic Flow
LBM	Lattice Boltzmann Method
REV	Representative Elementary Volume

Greek symbol	Unit	Description
β	-	Artificial compressibility parameter
ε	-	Dielectric constant
ε_0	$C \cdot (V \cdot m)^{-1}$	Permittivity of the vacuum
ζ	V	Zeta potential
ζ'	V	Modified Zeta potential
η	-	Numerical constant
κ	-	Debye length
λ	m	Brinkmann screening length
μ	$Pa \cdot s$	Viscosity
ϕ	V	External electric potential
Φ	-	Porosity
ρ_f	$kg \cdot m^{-3}$	Fluid density
ρ_e	$C \cdot m^{-3}$	Net charge density
ρ_{eff}	$C \cdot m^{-3}$	Effective charge density
σ	$S \cdot m^{-1}$	Electrical Conductivity
τ	-	Tortuosity
ψ	V	EDL potential

Subscript symbol	Description
B	Brinkmann
$chan$	Channel
$conv$	Convective
cp	Charged particles
cw	Charged walls
d	Darcy
$diff$	Diffusive
e	Net
eff	Effective
f	Fluid
ref	Reference
p	Particle
w	Walls

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