Proceedings of the 24th UK Conference of the Association for Computational Mechanics in Engineering
31 March - 01 April 2016, Cardiff University, Cardiff

FINITE ELEMENT MODELLING OF ELECTRO-OSMOTIC FLOW IN POROUS MEDIA

***Simona Di Fraia[1,2], Nicola Massarotti[1] and Perumal Nithiarasu[2]**

[1]Dipartimento di Ingegneria, Universitá degli Studi di Napoli "Parthenope", Napoli, 80143, Italy
[2]Zienkiewicz Centre for Computational Engineering, College of Engineering, Swansea University, Swansea, SA1 8EN, UK

*simona.difraia@uniparthenope.it

ABSTRACT

Electro-osmotic flow (EOF) in microchannels with and without porous media has been analysed in this work. The effect of the charge of solid particles on EOF has been taken into account by introducing an equivalent reference length into the equation that governs the static potential distribution. External electric field and internal potential have been determined by solving the Laplace and Poisson-Boltzmann equations, respectively. Their effect has been introduced into the Navier-Stokes equations to simulate fluid flow and heat transfer due to electro-osmosis. The set of equations that describes the problem has been solved using the finite element method combined with the characteristic-based split algorithm.

Key Words: *Electro-osmosis; Porous materials; Microscopic approach; CBS.*

1. Introduction

Electro-osmosis is important due to its applications in several fields of biology and engineering, mainly for pumping, cooling, mixing and separation processes. In Electro-Osmotic Flow (EOF) driven systems a solid surface, in contact with an electrolytic solution, becomes a charged surface. Consequently, the ions in the solution form of a high concentration region close to the solid surface, called Electrical Double Layer (EDL). When an external electric field is applied, the ions of the EDL move, dragging the nearby ions with them. In standard channel flow applications, the active surfaces are the channel walls. In channels filled with electrolyte saturated porous media, the boundaries of solid particles also contribute to electro-osmosis.

EOF in micro- and nano- fluidic systems has been widely investigated, experimentally and numerically. On the contrary, EOF in porous media is still not clearly analysed [1]. Experimental data are difficult to collect, due to the small scales, while for numerical modelling different approaches have been used and in most cases the results have not been validated against experimental results. In addition, several simplifying hypotheses have been considered in modelling EOF in porous media. To better understand EOF through porous media, a well defined porous medium is studied in the present work by using a microscopic approach. The flow results obtained for EOF through a of porous medium are compared against standard microchannel EOF without porous medium.

2. Mathematical model and solution procedure

The Laplace equation for the external applied potential and a non-linear Poisson-Boltzmann equation for the internal potential have been solved explicitly, by adding a pseudo time term. Their effect, responsible for EOF, has been implemented into the source term of the momentum equation of Navier-Stokes equations [3]. The Laplace and Poisson-Boltzmann equations are presented in non-dimensional form as

- *Laplace equation*

$$\frac{\partial^2 \phi^*}{\partial x_i^{*2}} = 0 \tag{1}$$

- *Poisson-Boltzmann equation*

$$\frac{\partial^2 \psi^*}{\partial x_i^{*2}} = -\left(\kappa L_{ref}\right)^2 \sinh\left(\frac{\psi^*}{T^*+1}\right) \tag{2}$$

where ϕ^* is the non dimensional applied external potential, ψ^* the non dimensional Electric Double Layer (EDL) potential (internal potential), κ is known as Debye-Huckel parameter, L_{ref} is the reference length and T^* is the non dimensional temperature. The Debye-Huckel parameter [2] is given as

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

where n_0 is the ionic number concentration in the bulk solution, z the valance of the ions, e the elementary charge, k_B the Boltzmann's constant, T is the reference temperature measured in kelvin, ϵ the dielectric constant of the electrolyte and ϵ_0 the permittivity of vacuum.
The parameter κL_{ref} used in Equation (2) represents the thickness of the EDL: it largely affects the internal potential distribution and consequently the flow profile within the channel. It appears that in the literature, the equation that governs internal potential distribution has not been modified to include the effect of porous media. This approach tends to underestimate the contribution of the charge of solid particles in the porous medium. Therefore, in the present work the authors have considered an equivalent reference length, assumed equal to the ratio between the area the channel occupied by the fluid and the length of the channel:

- in case of fluid $L_{ref,eq}$ corresponds exactly to the channel width, consistent with the quantity commonly used in previous works concerning EOF;
- for porous media the use of $L_{ref,eq}$ into Equation (2) should allow flow enhancement due to the charge of solid particles. An equivalent length as discussed previously is employed in the present study.

Fluid flow and heat transfer in standard micro-channels and through porous media have been analysed through the Navier-Stokes equations. They are given in their non-dimensional form as

- *Continuity equation*

$$\frac{1}{\beta^{*2}}\frac{\partial P^*}{\partial t^*} = -\rho^* \frac{\partial u_i^*}{\partial x_i^*} \tag{3}$$

- *Momentum equation*

$$\rho^*\left(\frac{\partial u_i^*}{\partial t^*} + \frac{\partial\left(u_i^* u_j^*\right)}{\partial x_j^*}\right) = -\frac{\partial p^*}{\partial x_i^*} + \frac{1}{Re}\frac{\partial^2 u_i^*}{\partial x_i^{*2}} + J \sinh\left(\frac{\psi^*}{T^*+1}\right)\left(\frac{\partial \phi^*}{\partial x_i^*}\right) \tag{4}$$

- *Energy equation*

$$\frac{\partial T^*}{\partial t^*} + u_i^* \frac{\partial T^*}{\partial x_i^*} = \frac{\alpha^*}{RePr}\frac{\partial^2 T^*}{\partial x_i^{*2}} + Jo\left(\frac{\partial \phi^*}{\partial x_i^*}\right) \tag{5}$$

where

$$Re = \frac{\rho_{ref} u_{ref} L_{ref}}{\mu}; \qquad J = \frac{2n_0 k_B T}{u_{ref}^2 \rho_{ref}}; \qquad Jo = \frac{1}{RePr}\frac{\sigma_{ref}}{k_{ref}}\frac{k_B^2 T_{ref}}{z^2 e^2};$$

The other non-dimensional quantities used in the above non dimensional form of equations are

$$x_i^* = \frac{x_i}{L_{ref}}; \qquad \phi^* = \frac{ze\phi}{k_B T}; \qquad \psi^* = \frac{ze\psi}{k_B T}; \qquad T^* = \frac{T - T_{ref}}{T_{ref}}; \qquad \rho^* = \frac{\rho}{\rho_{ref}};$$

$$u_i^* = \frac{u_i}{u_{ref}}; \qquad u_{ref} = \frac{E_x \epsilon \epsilon_0 \zeta}{\mu} \qquad t^* = \frac{t u_{ref}}{L_{ref}}; \qquad p^* = \frac{p - p_{ref}}{\rho_{ref} u_{ref}^2}; \qquad \beta^* = \frac{\beta}{u_{ref}};$$

where β is an artificial compressibility parameter [4]. Fluid flow and heat transfer equations have been solved by using finite element method combined with a fully explicit artificial compressibility-based CBS (Characteristic Based Split) scheme [5] to overcome the instability caused by the pressure term of the momentum equation.

The walls and any solid boundary have been assumed to be active with a prescribed non-dimensional zeta potential and to obey no-slip velocity boundary conditions. An applied external potential difference between the inlet and outlet has been considered and the normal velocity gradients have been assumed to be zero at both inlet and outlet. The computation has been started with prescribed zero velocity components as initial condition. A 2D unstructured mesh refined near all solid boundaries to capture the rapid change in both internal potential and velocity has been used. A mesh sensitivity study has been carried out in order to find grid insensitive results.

In order to assess the effectiveness of using porous media to enhance EOF, a comparison with standard channel flow applications has been carried out. Fluid flow and heat transfer through porous media have been analysed through the so-called microscopic approach [6], that provides details of the fields for the quantities of interest at particle level. The analysis has been focused on the improvement in EOF due to the use of the equivalent reference length proposed in the present work.

3. Results and Discussions

A silicon micro-channel 30 μm in diameter characterized by an aspect ratio of 10, with deionized water as working fluid, has been considered. Porous media have been investigated at the pores level, with solid particles assumed to be circular in shape. Two cases have been considered:

- particles arranged in line, diameter equal to 50% of the channel diameter;
- staggered particles, diameter equal to 30% of the channel diameter.

A non-dimensional external potential difference of 2 000 was prescribed between the inlet and outlet of the channel. The non-dimensional zeta potential value of -3, corresponding to $-75mV$, has been considered for both the channel walls and the solid particles.

The distribution of the internal potential is shown in Figure 1, where only part of the whole domain is reported here to clearly view the details.

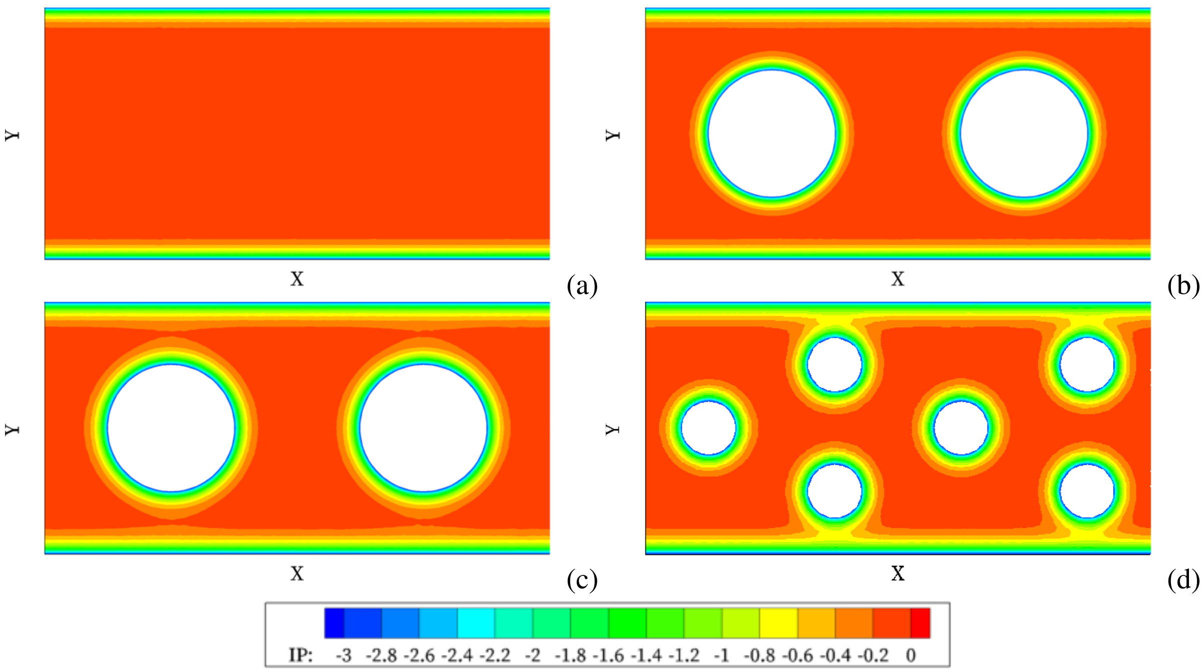

Figure 1: Internal potential (IP) distribution: standard fluid channel (a) and porous channel with in line particles with standard channel width (b) and with the proposed $L_{ref,eq}$ (c), staggered particles with the proposed $L_{ref,eq}$ (d).

For EOF in porous media with in line particles two cases have been considered: firstly, the equation that governs internal potential distribution has not been modified, and the width of the channel has been used (Figure 1 b), secondly the equivalent reference length proposed by the authors has been considered (Figure 1 c). The results obtained highlight that, by using $L_{ref,eq}$ instead of the whole width of the channel, the effect of the charge of solid material in the narrow region between the channel wall and the particle is taken into account. The internal potential distribution plays a fundamental role on the velocity distribution and consequently on the flowrate. The effect of using the proposed equivalent length on the outlet velocity profile is illustrated in Figure 2. As seen, the equivalent width used substantially increases the flow rate when porous media have been considered.

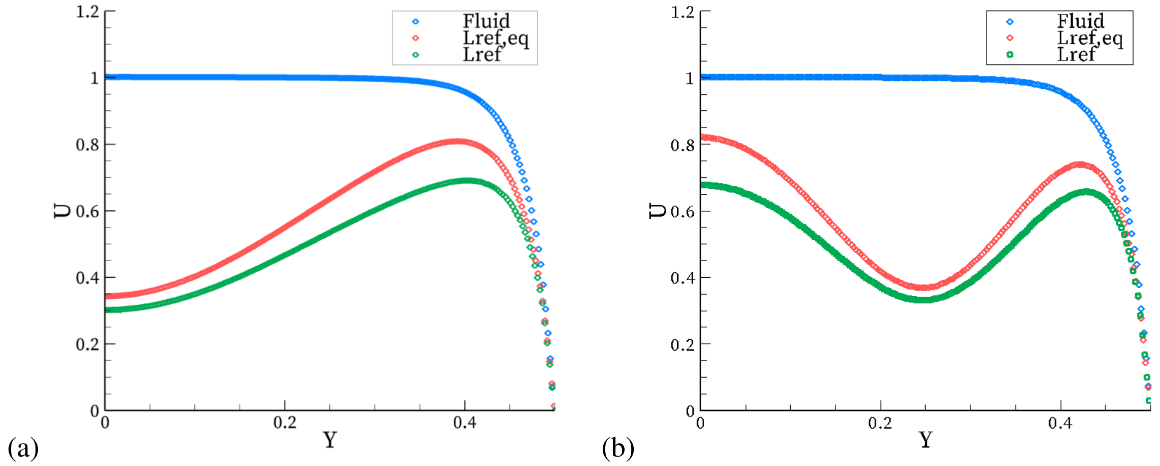

Figure 2: Outlet velocity profiles: comparison between fluid and in line particles (geometry b-c of Figure 1) (a), staggered particles (geometry d of Figure 1) (b).

4. Conclusions

Electro-osmotic flow through porous media has been studied and compared to the standard channel flow applications. For modelling porous media flow an equivalent reference length has been employed. The use of this parameter allows us to take into account the influence of the charge of solid particles on the internal potential distribution and capture the behaviour in the narrow regions between solid particles and channel walls. The results of this study will be used by the authors to define the parameters for modelling EOF in porous media by using a macroscopic approach.

References

[1] B. Li, W. N. Zhou, Y. Y. Yan, C. Tian. Evaluation of electro-osmotic pumping effect on microporous media flow. *Applied Thermal Engineering*, 60, 449–455, 2013.

[2] N. A. Patankar, H. H. Hu. Numerical simulation of electroosmotic flow. *Analytical Chemistry*, 70(9), 1870–1881, 1998.

[3] R. J. Yang, L. M. Fu, Y. C. Lin. Electroosmotic flow in microchannels. *Journal of colloid and interface science*, 239(1), 98–105, 2001.

[4] P. Nithiarasu. An efficient artificial compressibility (AC) scheme based on the characteristic based split (CBS) method for incompressible flows. *International Journal for Numerical Methods in Engineering*, 56(13), 1815–1845, 2003.

[5] P. Nithiarasu, R. W. Lewis, K. N. Seetharamu. *Fundamentals of the Finite Element Method for Heat and Mass Transfer*, John Wiley and Sons, 2016.

[6] N. Massarotti, P. Nithiarasu, A. Carotenuto. Microscopic and macroscopic approach for natural convection in enclosures filled with fluid saturated porous medium, *International Journal of Numerical Methods for Heat and Fluid Flow*, 13(7), 862–886, 2003.