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Theoretical modelling of electrokinetic flow in microchannel networks

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Abstract

This work deals with the description of electrokinetic flow in microfluidic networks involving multiple channels intersections. A generalized one-dimensional modelling is carried out to predict flow rate and electric current in each branch of the network, as a function of applied electric potentials and pressure gradients. Mathematical derivations ground on thermodynamic formalisms for electrokinetic phenomena, and takes into account the characteristics of every channel and circulating fluid in the system. The coefficients that relate driving forces and conjugated flows are derived for both slit and cylindrical microchannels, with arbitrary values of surface potential and electric double layer thickness. Calculations are used to rationalize typical operations performed in analytical devices that consist of well-defined microchannel networks. The modelling suggested also provides an accurate basis to study fundamental aspects of electrokinetic phenomena in microfluidic systems.

Keywords: Electrokinetic flow; Microchannel networks; Microfluidics; Analytical devices

1. Introduction

Analytical microfluidic devices, as those currently used in chemical, biological and medical applications, basically consist of different networks of microchannels that connect chambers and reservoirs [1–5]. The architecture of these networks may be more or less complex, involving the basic units drawn schematically in Fig. 1. In order to manipulate the transport of fluids, microchannels are generally subjected to pressure gradients, electric fields, or a combination of the two. Therefore, in view of technological applications, reliable models are necessary to describe the coupled flows of matter and electricity developed in every branch of the network. For this purpose, a sound understanding of the mechanisms governing electrokinetic phenomena in microfluidic systems is required [12].

Detailed treatments of microchannel networks involve the modelling of electrokinetic and transport phenomena in the whole system, considering effects in two and three dimensions, which demands important computational efforts [7,9,12–14]. Nevertheless, if microchannels are sufficiently slim, flows are fully developed and two-dimensional effects are present near the channel intersections only (Reynolds numbers are normally lower than 1 in microchannels [15]). Under these circumstances, one-dimensional modelling applies as a first approximation. This approach greatly simplifies calculations and still provides valuable information to design and operate integrated microfluidic systems. Thus, compact models have been derived by emulating electrical circuits [6,9,16,17]. Although useful in practical manipulations, these models are limited to micro-scale channels and relatively high ionic concentrations, as calculations assume negligibly thin electric double layers (EDL) in relation to channel cross-sectional size. The effect of heterogeneities in channel characteristics is also underestimated. Addressing these issues, a more complete analysis has been proposed to model single junction networks of cylindrical capillaries [8]. However, for the particular case of electro-osmotic flow (EOF), equations reported apply for channel ends exposed to atmospheric pressure only.

It should be observed that the simultaneous presence of both electric potential and pressure gradients need to be considered, because these conjugated forces can rarely be decoupled. In systems driven solely by pressure, streaming phenomena occur when microchannels contain interfacial charge, and hence the electrokinetic ζ-potential is present (see, for instance [18]). Conversely, in systems driven by EOF, pressure differences take place if the ζ-potential varies from one branch to another

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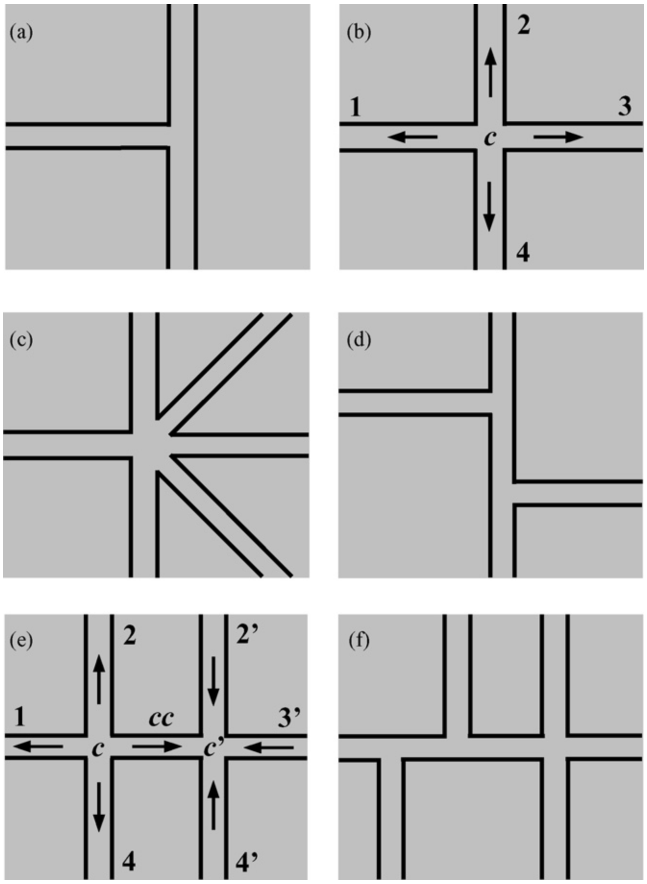

Fig. 1. Schematic representation of different microchannel networks: (a) T-shaped [6], (b) cross-shaped [7], (c) multi-branch [8], (d) double-T [9], (e) double-cross [10], and (f) multi-junction [11]. References cited above are some of several examples found in the recent literature. In particular, schemes (b) and (e) include the nomenclature used here to identify branches and junctions in calculations. Also in these schemes, arrows indicate the positive direction of the flow.

[13,19,20]. Further, even when channel ends are open to atmosphere, pressure gradients arise due to differential meniscus curvatures generated in the reservoirs located at channel ends [21,22], or due to unequal fluid heights, for example, when the plate containing the network is not placed normal to gravity [21,23]. As a last point, it is worth noting that novel applications combine EOF and pressure-driven flow in the same device [24].

In this context of analysis, the present work discusses a generalized modelling of the one-dimensional, steady state, electrokinetic flow in microchannel networks. Systems containing multiple junctions and channels with different characteristics (geometry, surface properties, circulating fluid) are taken into consideration. Calculations are aimed to assess the flows of matter and electricity in each branch of the network, as a function of applied electric potentials and pressure gradients. The modelling is performed in the framework of Onsager relations for electrokinetic phenomena [25]. In this sense, the work deals with a particular, extended application of the general formalism revised in [26] and, more specifically, in [27]. In fact, here the coefficients entering the conductance matrix, which relates driving forces and conjugated flows, are derived for both axial and plane-symmetric electrokinetic flows, with arbitrary values of ζ-potential and EDL thickness. In addition, these results are then used to interpret typical operations carried out in well-defined microfluidic networks.

The paper is organized as follows: in Section 2, the equations required to predict the flow rate and the electric current in networks of microchannels are outlined. These equations include coupling coefficients that must be deduced from the governing equations of electrokinetic flow. For the purposes, theoretical concepts are overviewed in Section 3. Then in Section 4, the coefficients are derived in a general form that involves cylindrical and slit microchannels. In particular, analytic expressions are given for symmetric electrolyte solutions flowing through slit channels with relatively low surface potentials (Appendix A). Finally, in Section 5, some examples are considered to illustrate the capability of the approach to explain situations of practical interest.

2. Conjugated flows in microchannel networks

2.1. Single microchannels

The aim of this section is to quantify the flow rate Q and the electric current I developed in straight microchannels, which contain interfacial charge and the associated EDL of ions in solution. The driving forces are electric potential and pressure differences between the ends of the channels, ΔV and ΔP, respectively. In steady state and isothermal conditions, the simultaneous flows are described by Onsager relations [25]:

$$Q = L_{11}\Delta P + L_{12}\Delta V, \tag{1}$$

$$I = L_{21}\Delta P + L_{22}\Delta V, \tag{2}$$

where L_{11}, L_{12}, L_{21}, and L_{22} are coupling coefficients that depend on the characteristics of both microchannel and fluid, as it will be described in detail in Sections 3 and 4. In particular, the matrix of coefficients is symmetric, i.e., $L_{12} = L_{21}$, thus satisfying Onsager fundamental theorem [25–27]. Eqs. (1) and (2) assume that there are no concentration gradients in the axial direction, which is a good approximation provided the channels are sufficiently slim. When osmotic effects are important, an additional term is involved in these equations [26–28].

2.2. Single junction networks

Given networks with one channel intersection, like those shown in Fig. 1a–c, it is of interest to predict the flow rate and the electric current in every branch. For this purpose, the following conservation equations are written:

$$\sum_{i=1}^{N} Q_i = 0, \tag{3}$$

$$\sum_{i=1}^{N} I_i = 0, \tag{4}$$

where sub index i refers to branch number and N is the total number of branches in the network (for example, $N = 4$ in Fig. 1b). Eq. (3) derives from a simple mass balance for incompressible