Numerical modeling of surface reaction kinetics in electrokinetically actuated microfluidic devices

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HIGHLIGHTS

- Surface reactions in electrokinetically actuated microfluidic devices are studied.
- Governing equations are solved using a finite difference based numerical procedure.
- A concentration wave is observed for sufficiently long microchannels.
- Modeling a reactor as a slit leads to an underestimation of the saturation time.

GRAPHICAL ABSTRACT
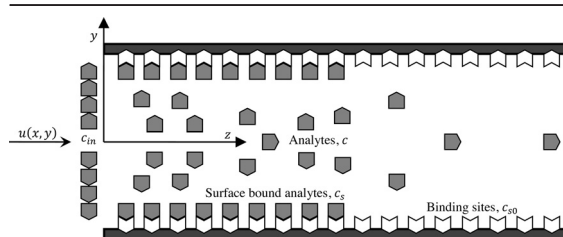
ABSTRACT

We outline a comprehensive numerical procedure for modeling of species transport and surface reaction kinetics in electrokinetically actuated microfluidic devices of rectangular cross section. Our results confirm the findings of previous simplified approaches that a concentration wave is created for sufficiently long microreactors. An analytical solution, developed for the wave propagation speed, shows that, when normalizing with the fluid mean velocity, it becomes a function of three parameters comprising the channel aspect ratio, the relative adsorption capacity, and the kinetic equilibrium constant. Our studies also reveal that the reactor geometry idealized as a slit, instead of a rectangular shape, gives rise to the underestimation of the saturation time. The extent of this underestimation increases by increasing the Damkohler number or decreasing the dimensionless Debye–Hückel parameter. Moreover, increasing the values of the Damkohler number, the dimensionless Debye–Hückel parameter, the relative adsorption capacity, and the velocity scale ratio results in lower saturation times.

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1. Introduction

With the advent of lab-on-a-chip (LOC) devices, electroosmosis has featured as a predominant mechanism for flow actuation.

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Electroosmotic micropumps have many advantages over the other types of micropumps. For example, unlike the classical pressure-driven micropumps involving moving components, the electroosmotic pumps have no moving parts and are simpler to be designed and fabricated [1,2]. Moreover, these pumps are bidirectional and capable of generating constant and pulse free flows with flow rates well suited to LOC systems [3].

The fundamental origin of electroosmotic transport lies in the fact that when a surface is brought into contact with an electrolyte solution, it usually takes a net charge [4]. Due to the
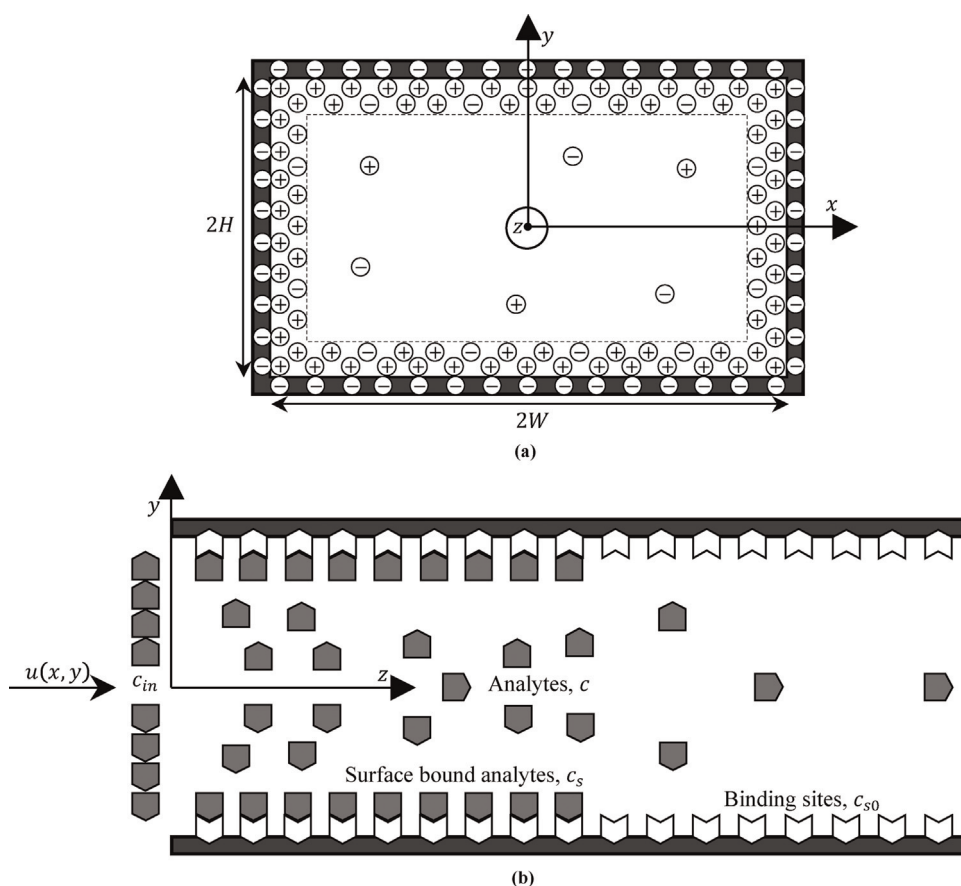
Fig. 1. Schematic representation of an electrokinetically driven microreactor (a) transverse view including the EDLs between the channel inner wall and the dashed lines and (b) lateral view containing the reactive components.

electroneutrality principle, the liquid takes on an opposite charge in the electric double layer (EDL) near the surface. The electric double layer, shown schematically in Fig. 1, contains an immobile inner layer and an outer diffuse layer [5]. If an electric field is applied tangentially along the surface, a force will be exerted on the ions within the mobile diffuse electric layer, resulting in their motion [6]. Owing to viscous drag, the liquid is drawn by the ions and, therefore, flows tangential to the surface.

Microreactors are one of the essential components of the LOC devices. As compared to their macroscale counterparts, micro-reactors have many unique advantages. For example, decrease in the length scales in these devices gives rise to larger concentration gradients, thereby increasing the mass transport. Moreover, the higher surface to volume ratios at microscale result in higher reaction rates for the systems in which the reaction takes place on the surfaces. In addition, due to the fact that the increase in throughput in microreactors is achieved by a numbering-up approach rather than by scaling-up, higher flexibility is achieved in adapting production rate to varying demands, since a certain number of systems can be switched off or further systems may be simply added to the production plant [7].

Microreactors are generally divided into homogenous and heterogeneous categories. In the former, reaction takes place within the solution. However, in the heterogeneous reactors, one of the reactants is immobilized on a solid surface and the other reactant is brought close to the surface by the carrier fluid [8]. In both cases, the mass transport process can be considered as a subcategory of solute dispersion with chemical reaction. By tracking the literature, one may come across the work of Taylor [9], as one of the landmark research works on solute dispersion. He provided a description of the cross-sectional-area averaged axial

advective and diffusive transport of a passive Brownian tracer particle inside a tube with laminar flow and impermeable walls in 1953. Since then, this method, and also its modified versions developed by other researchers [10–12], have been called Taylor dispersion theory in the literature. The first work extending the dispersion problem to the situations containing surface reactions was performed by Sankarasubramanian and Gill [13]. They developed analytical solutions for miscible dispersion in laminar flow inside a circular tube in the presence of irreversible first order reactions at the wall. Adopting the Taylor dispersion theory, Barton [14] extended the work of Sankarasubramanian and Gill [13] by considering reactive solutes.

Unlike the types of reactions presumed in the aforementioned research works, the reactions that take place in biological applications are mostly reversible. One of the first attempts in modeling the reversible surface reactions in biological devices was made by Glaser [15]. He numerically studied the kinetics of binding and dissociation between a soluble analyte and an immobilized ligand on or near a surface. This work was followed by a long line of research works on surface reaction kinetics in biomicrofluidic devices [8,16–24], all of them considering a pressure driven pumping mechanism. As for electrokinetically driven micro-devices, the relevant studies are more recent. About a decade before, a numerical analysis of the thermal effect on electroosmotic flow and electrokinetic mass transport in microchannels was reported by Tang et al. [25]. Analytical solutions for the rate of DNA hybridization in a microchannel in the presence of pressure driven and electroosmotic flows were presented by Das et al. [26] by considering a linear bulk concentration gradient. This research group also published the results of a numerical study of coupled momentum, heat, and solute transport during DNA hybridization