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# Electrokinetic energy conversion efficiency analysis using nanoscale finite-length surface-charged capillaries

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ABSTRACT

Electrokinetic power generation efficiency using a two-dimensional axisymmetrical model is numerically investigated. A finite-length nanoscale surface-charged cylindrical capillary with reservoirs connected at the capillary ends is considered as the physical domain. The Navier–Stokes, Laplace, Poisson, and Nernst–Planck equations are solved simultaneously to obtain the fluid flow, electrical potential, ion concentration and electrical current in the flow field. The energy conversion efficiency predicted using a one-dimensional model assuming an infinitely long channel, Boltzmann ion distribution and equal ionic electrical mobility is also carried out and compared with the two-dimensional result.

The two-dimensional model results show that the electrostatic potential gradient resulting from the concentration changes at the capillary entrance and exit and fluid flow produce a conductive current that reduces the total current in the flow field. The conductive current due to the electrostatic potential gradient increases with the decrease in electrolyte bulk concentration and increase in surface charge density. This results in nonlinear variations in the electric current–voltage curve and maximum conversion efficiency as functions of the surface charge density and dimensionless Debye length when the electrolyte bulk concentration is low. Comparison of the maximum efficiencies predicted from one- and two-dimensional models indicates that the one-dimensional model is valid only when the dimensionless Debye length is large and the surface charge density is small because the electrostatic potential gradient is neglected. The two-dimensional model also predicts that optimum maximum energy conversion efficiency can be obtained when the dimensionless Debye length is equal to 2 and its magnitude increases with the increase in surface charge density.



## 1. Introduction

Because of the developments in recent microfabrication technology, micro or nanoscale channels have become available, playing an important role in many engineering applications. For example, fluid transport in nanoscale fluidic systems by applying an external electrical field is used for chemical and biological analyses in the lab-on-a-chip devices [1–3]. Besides chemical and biological analyses, micro and nanoscale fluidic system applications in energy conversion based on electrokinetic effects have recently gained much interest in the research society because of the demand for finding new and environmental-friendly energy resources [4,5].

The electrokinetic energy conversion principle utilizes two fundamental electrokinetic effects: the streaming potential and electroosmosis. These two phenomena rely on the existence of an electrical double layer (EDL) near a channel wall. The theories regarding the formation of EDL, electroosmosis and streaming potential are well documented in several textbooks [6–8]. This is based on the fact that most surfaces are electrically charged when they are brought into contact with a polar medium such as an aqueous electrolyte. Because of the charged surface, preferentially distributed counter-ions and co-ions are created near the surface. The ion distribution combined with random thermal motion results in EDL formation. As the fluid flow is driven by an externally applied pressure gradient, the fluid flow carries the ions to the channel downstream. The charge transport results in an electric current, known as the streaming current. The charge polarization due to accumulated ions at the channel downstream creates an electrical potential difference between the channel ends and a conductive current with a direction opposite to the flow direction. The electrical potential difference is termed the streaming potential because it is created by the fluid flow. The streaming potential theory has recently been applied to build an electric power generation unit since the maximum streaming potential can be regarded as an open circuit potential (or the electromotive force) similar to that in an electrochemical cell [9–14]. Because of this similarity, electric power generation based on the streaming potential theory may be termed the "Electrokinetic Cell" (EK cell).

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**Nomenclature**

| | |
|---|---|
| $a$ | radius of cylindrical capillary (m) |
| $A_R$ | radius of computational domain in reservoirs (m) |
| $c_0$ | bulk electrolyte molar concentration, M (mol $L^{-1}$) |
| $D$ | molecular diffusivity ($m^2\ s^{-1}$) |
| $F$ | Faraday constant (96,500 C $mol^{-1}$) |
| $G$ | hydrodynamic conductance ($m^3\ Pa^{-1}\ s^{-1}$) |
| $L$ | length of cylindrical capillary (m) |
| $L_R$ | length of computation domains in reservoirs (m) |
| $m$ | electrical mobility (mol s $kg^{-1}$) |
| $M$ | streaming conductance (S) |
| $N$ | number of ions in the flow field |
| $p$ | pressure (Pa) |
| $P_{in}$ | input pumping power (W) |
| $P_{out}$ | output electric power (W) |
| $Q$ | flow rate ($m^3\ s^{-1}$) |
| $R$ | universal gas constant (8.314 J $mol^{-1}\ K^{-1}$) |
| $S$ | electrical conductivity (S) |
| $T$ | fluid temperature (K) |
| $\vec{V}$ | fluid flow velocity vector |
| $z$ | valence of ion |
| $Z$ | figure of merit of energy conversion |

*Greek letters*

| | |
|---|---|
| $\Lambda$ | electrolyte electrical conductivity (S $m^{-1}$) |
| $\varepsilon$ | dielectric permittivity, |
| $\varepsilon_0$ | permittivity of vacuum ($8.854 \times 10^{-12}$ C $V^{-1}\ m^{-1}$) |
| $\phi$ | externally applied voltage (V) |
| $\eta$ | energy conversion efficiency |
| $\mu$ | fluid viscosity (Pa s) |
| $\rho_e$ | net charge density (C $m^{-3}$) |
| $\sigma$ | surface charge density (C $m^{-2}$) |
| $\psi$ | electrostatic potential due to surface charge (V) |

*Subscript*

| | |
|---|---|
| $i$ | $i$th ion |
| max | maximum value |
| 1 | inlet reservoir |
| 2 | outlet reservoir |

From thermodynamic point of view, the EK cell can be viewed as an energy conversion process. The input power is the pumping power (product of pressure difference applied and flow rate) and the output is the electrical power (product of streaming potential created and electric current). A pioneering study dealing with electrokinetic energy conversion is the work of Osterle [15]. Based on Osterle's work one-dimensional analysis of electrokinetic energy conversion thermodynamic efficiency has been reported in several studies [13–14,16]. The one-dimensional model is based on the infinitely long channel length, equal ion diffusivity and mobility, and Boltzmann ion distribution assumptions. These assumptions may lead to under or over-predicted energy conversion efficiency.

In order to raise the energy conversion efficiency using the electrokinetic effect, a flow field containing many flow passages must be employed to increase the electric current. These multiple channel structures can be obtained through microfabrication technology, chemical synthesis or natural structures [9–10,17]. In general, these microstructures can be viewed as a charged porous media as they are in contact with a polar medium. Because of the structural characteristics, the charged porous media can be considered as composed of an array of identical parallel charged cylindrical capillaries with micro or nanoscale size. The charge inside the porous media can be considered uniformly distributed on the capillary walls with a certain charge density. From this point of view, it is more appropriate to consider the channel in the energy conversion unit as a charged cylindrical capillary instead of a planar slit or rectangular channel, as investigated in the studies of Daiguji et al. [11–12] and van der Heyden et al. [13–14].

In this study a two-dimensional EK cell model is established and solved numerically. A nanoscale finite-length surface-charged cylindrical capillary including the inlet and outlet reservoirs is considered as the physical domain [11–12,18]. The fundamental equations governing the fluid flow, multi-ion transport and electrical potential distribution are solved simultaneously without the assumptions made in the one-dimensional model. The thermodynamic efficiency results obtained from both the one- and two-dimensional models are compared and discussed.

## 2. Physical and mathematical models

As shown in Fig. 1, we consider a cylindrical capillary having a radius of $a$ and a length of $L$. Without loss of generality, the capillary wall is considered negatively charged with a surface charge density of $\sigma$. The ends of the capillary are connected to inlet and outlet reservoirs which are assumed to be infinitely large compared with the capillary size. We assume that an aqueous salt solution with bulk molar concentration $c_0$ entirely fills the system and the system is initially in equilibrium. The physical domain considered in this study is the same as that in the studies of Daiguji et al. [11–12] except that the planar slit is replaced by a cylindrical capillary.

For the EK cell operation, fluid flow is driven by an applied pressure difference and creates an electrical potential difference. This can be described using the pressure and voltage differences between the inlet and outlet reservoirs. As shown in Fig. 1, pressure and potential in the inlet and outlet reservoirs are denoted as $\phi_1$, $p_1$, $\phi_2$, $p_2$, respectively. The externally applied pressure difference is $\Delta p = p_2 - p_1 < 0$ and the created streaming potential is $\Delta\phi = \phi_2 - \phi_1 > 0$. Under such applied pressure difference, the fluid flow direction is from the inlet reservoir to outlet reservoir.

### 2.1. One-dimensional model of EK cell

The one-dimensional EK cell model has been given in several investigations [13–14,16]. A brief summary based on the results reported by Xuan and Li [16] is given below. Based on the Onsager reciprocal theorem, the relations between the flow rate $Q$, electric current $I$, pressure difference $\Delta p$, and the voltage difference $\Delta\phi$ for the flow with electrokinetic effect through a channel with any cross-sectional shape can be written as,

$$Q = G(-\Delta p) + M(-\Delta\phi) \quad (1)$$

$$I = M(-\Delta p) + S(-\Delta\phi) \quad (2)$$

where $G$ represents the hydrodynamic conductance, $M$ characterizes the electroosmotic flow rate in Eq. (1) and the streaming

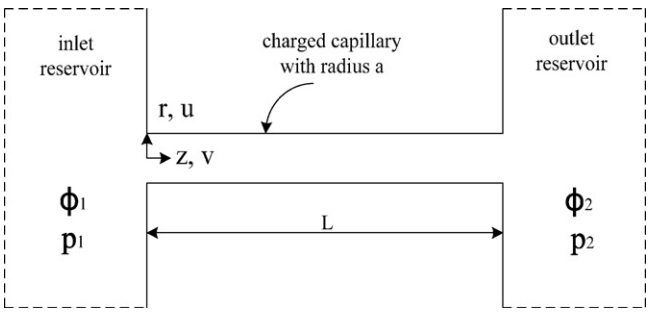


**Fig. 1.** Schematic of the physical system.