



# A microfluidic pumping mechanism driven by non-equilibrium osmotic effects

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## ABSTRACT

A mechanism is presented which drives a fluid flow using two chemically reacting molecular species and osmotic effects. For concreteness the mechanism is discussed in the context of a tube which at each end has a capping membrane which is permeable to the fluid but impermeable to the two molecular species. The chemical reactions occur at sites embedded in the capping membrane. Labeling the two chemical species *A* and *B*, at one end the reactions split each molecule of species *B* into two molecules of species *A*. On the other end two molecules of species *A* are fused together to form a single molecule of species *B*. A mathematical model of the solute diffusion, fluid flow, and osmotic effects is presented and used to describe the non-equilibrium steady-state flow rate generated. Theoretical and computational results are given for how the flow rate depends on the relative diffusivities of the solute species and the geometry of the system. An interesting feature of the pump is that for the same fixed chemical reactions at the tube ends, fluid flows can be driven in either direction through the tube, with the direction depending on the relative diffusivities of the solute species. The theoretical results are compared with three-dimensional numerical simulations of the pump.

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## 1. Introduction

In recently proposed technological devices and in many biological systems, gradients in fluid pressure are generated by osmotic effects to drive a flow [2–9]. Osmosis occurs when solute molecules immersed in a fluid are confined within a region delineated by a boundary less permeable to molecules of the solute than the fluid. When the boundary in question is rigid, this results in a pressure exerted on the confining boundary, which exceeds that of the solvent pressure, with a dependence on the concentration of the solute and the temperature of the system. This additional pressure in the system is referred to as the “osmotic pressure”. For systems in which the confining boundary is flexible, swelling can also occur as water flows into the confining region, increasing its volume until the elastic stresses in the flexible walls have built up enough to balance the osmotic pressure [10,8], which meanwhile has been somewhat reduced by the dilution of the confined solute.

Various microfluidic pumps and actuator devices have been proposed which exploit osmosis either making use of swelling structures or electrostatic effects [1,6,7,11]. In [6,7,11] osmotic swelling is exploited to generate forces in a microactuator or to

generate deformations in vessels containing a drug for delivery. In [8,9] propulsion mechanisms are proposed which make use of a concentration gradient in the environment which induces unbalanced osmotic pressures on a small particle or lipid vesicle. In [1] an electrostatic field drives a fluid flow through a flux of ions which develops in a boundary layer of the charged wall of the pump.

In cell biology, osmotic effects play an important role. Within cells and organelles there are high concentrations of charged proteins and counter-ions. The effects of osmotic pressure must be actively mitigated by ion pumps or other means to avoid excessive swelling which could burst the cell or organelle [12,13]. Regulation of the volume of such structures can be used to drive an in-flux or out-flux of fluid which may be important in many biological processes in the cell [14,3]. Osmotic effects are also thought to play an important role in tissues of epithelial cells in the kidney, liver, and intestine in which a large volume of fluid is processed each day. A number of pumping mechanisms have been proposed that make direct use of osmotic effects [15,3,16,12,17,4,18,5].

In the systems mentioned above an osmotic pressure gradient is set up either by active pumping of solute molecules from a large external store into a confined region or by an external electrostatic field. In the present work a pumping mechanism is discussed which does not require an external store of solute molecules or electrostatic effects. In the mechanism proposed here the solute molecules are recycled in the process that sets up the osmotic pressure gradient.

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A variety of approaches have been taken to model osmotic phenomena ranging from thermodynamic relations to microscopic statistical mechanical descriptions [19–24,8,9]. The classical work by van 't Hoff gives an equilibrium thermodynamic law for macroscopic osmotic pressure in terms of the overall temperature of the system and the difference in concentration of the solute which is confined by a semi-permeable membrane with that of the solute in the outside bulk solvent [24]. A microscopic approach can also be taken based on the mechanics of the solute–wall interactions which does not necessarily require the system to be in thermodynamic equilibrium [19,20].

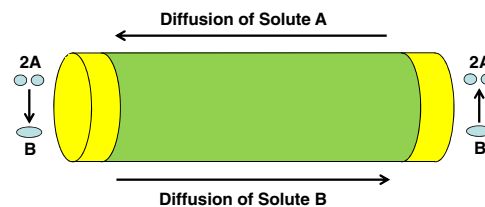
In this paper we shall take a microscopic approach to the study of how the osmotic pressure arises in the non-equilibrium setting of active chemical reactions and fluid flows. We shall then perform analysis to obtain a description of the osmotic pressure of the pump by taking the limit in which the solute confining potentials at the semi-permeable membranes only act in a very small boundary layer of the capping ends of the pump, which corresponds to what we term the “hard-walled limit” [19]. This description is then used to carry out three-dimensional numerical simulations of the microfluidic pumping mechanism using a variant of the finite volume method of [25] and the immersed boundary method [26].

The paper is organized as follows. In Section 2, the pumping mechanism is discussed. To demonstrate the mechanism, a mathematical model of a pump with cylindrical geometry is formulated in Section 3. To obtain an analytically tractable set of equations, reductions are then made to the model in Section 4 and theoretical predictions for the steady-state pumping rate are given. Numerical methods for the full system of equations for the osmotic phenomena which accounts for general confining potentials, the fluid flows, and chemical reactions are presented in detail in Section 5. The specific numerical methods used for the full three-dimensional model of the osmotic pump are then presented and the results of simulations are discussed in comparison to the theoretical predictions made from the reduced model.

## 2. The pumping mechanism

For concreteness we shall discuss the mechanism in the context of a system which has two solute species  $A$  and  $B$  which are assumed to be confined to the interior of a cylindrical tube. Two planar cross-sections of the tube are spanned by membranes which are permeable to solvent but impermeable to the solute species  $A$  and  $B$ . The curved cylindrical walls of the tube are impermeable to solute and solvent alike. For the purpose of our analysis we shall regard the entire cylindrical pump as being embedded in a longer tube which is bent to reconnect with itself so that solvent fluid is re-circulated. We shall assume that this is done in such a manner that the curvature has a negligible effect on the solvent flow. More general geometries and additional solute species could of course be considered to obtain other variants of the proposed pumping mechanism.

The chemistry of the system will occur only in the vicinity of the membranes spanning the cross-section of the tube. Since these membranes act like “caps” for the cylindrical region defined between the cross-sections we shall refer to the semi-permeable membranes as “capping membranes”. The capping membrane at one end of the tube contains reaction sites (embedded enzymes) at which a solute molecule of species  $B$  is split into two solute molecules of species  $A$ . At the other end of the tube is a capping membrane with embedded reaction sites which combine two molecules of species  $A$  to form a single molecule of species  $B$ . We remark that even though one of the chemical reactions is the reverse of the other, an energy source is needed to power the pump in general. This is because the chemical reactions are localized and not directly coupled, with one reaction occurring independently at



**Fig. 2.1.** Pump schematic. On the left end of the tube two molecules of species  $A$  bind to form a single molecule of species  $B$ . When molecules of species  $B$  diffuse or are transported by the fluid to the right end of the tube the molecule of species  $B$  is split into two molecules of species  $A$ . Throughout the chemical reactions the total number of elementary chemical units is conserved as either free species  $A$  molecules or as bound pairs which form a single molecule of species  $B$ .

one end of the tube, provided there are sufficient reactants, while the other reaction occurs independently at the other end of the tube.

Suppose for example that one of the chemical reactions, say  $B \rightarrow A + A$ , is strongly favored (for energetic and/or entropic reasons) under the prevailing conditions throughout the pump, and therefore requires only a catalyst to occur. Then no energy source is needed at the capping membrane where this reaction occurs. However, precisely because the  $B \rightarrow A + A$  reaction is favored, we cannot expect the reverse reaction  $A + A \rightarrow B$  to happen preferentially at the other capping membrane. For the reaction  $A + A \rightarrow B$  to occur requires an energy source. In an experimental system the chemistry might be realized by enzymes embedded in the membranes of the capping ends which derive energy from an auxiliary source such as hydrolysis of  $ATP$  molecules, see [27]. Another approach to obtain a similar effect as we shall discuss could be to utilize for ions or small molecules a form of “facilitated diffusion” for transport across the capping membranes which has different kinetics for the two membranes [13]. For a schematic of the pumping mechanism see Fig. 2.1.

At steady-state the system is expected to have an imbalance in the number of solute molecules at the opposing ends of the tube. Osmotic pressure differences at the ends of the tube are then expected to drive a fluid flow through the tube from the end with a greater number of solute molecules toward the end with fewer molecules. However, predicting features of this steady-state on intuitive grounds is made challenging given the coupling between the chemical reactions, transport by the fluid, and diffusion. As we shall discuss, the flow may be made to move opposite to the natural direction suggested by the chemical reactions by an appropriate choice of the relative diffusivities of the solute species.

## 3. A theoretical model of the pump

The geometry of the model system consists of a long tube having total length  $L^*$  and radius  $R$ . The pump will be embedded in this long tube and consist of a sub-segment of the tube of length  $L$  which is delimited by two semi-permeable membranes. We shall refer to this region as the “tube” of the pump. References to the “ends of the tube” will refer to the boundaries defined by the semi-permeable membranes. Throughout, the pump should be regarded as being embedded within a longer tube of length  $L^*$  which reconnects with itself to re-circulate the solvent fluid, which corresponds to periodic boundary conditions on the tube of length  $L^*$ .

To take into account how osmotic effects arise in the system, explicit solute–wall interactions are modeled through two conservative forces having potentials  $V_A$  and  $V_B$ , which act on the solute particles of species  $A$  and  $B$  respectively. To separate those forces acting on the solute inside the tube and those forces acting merely to confine solute particles to the tube, the geometry used in the mathematical model will consist of a slightly larger cylindrical tube having radius  $R + \xi$  and extending in length from  $[-\epsilon, L + \epsilon]$ .

For systems having purely confining forces this will be modeled by potentials  $V_A$  and  $V_B$  which are non-constant only outside of the tube of radius  $R$  and length  $L$ . The  $\xi$  and  $\epsilon$  parameters then specify the width of the boundary layers on which the confining forces act. To ensure that conservative forces indeed confine the solute to the extended tube, the potentials  $V_A$  and  $V_B$  are required to diverge over the boundary layer. This can be expressed by the following conditions which will be assumed throughout:  $V_A(L + h, y, z) \rightarrow \infty$ ,  $V_B(-h, y, z) \rightarrow \infty$ , as  $h \rightarrow \epsilon$ , and  $V_A(x, (R + r) \cos(\theta), (R + r) \sin(\theta)) \rightarrow \infty$ ,  $V_B(x, (R + r) \cos(\theta), (R + r) \sin(\theta)) \rightarrow \infty$  as  $r \rightarrow \xi$ , where  $x \in [-\epsilon, L + \epsilon]$ ,  $y^2 + z^2 < R^2$ , and  $\theta \in [0, 2\pi]$ . We remark that these confining potentials play a crucial role in the mechanism underlying the osmotic pressures of the system, which arise from the persistent confining forces exerted on the solute particles maintained in the boundary layer by diffusion. A detailed discussion of this mechanism is given in [19].

In the model the reactive membranes will be cross-sections of the tube located at  $x = 0$  and  $x = L$  and will be freely permeable to particles of the non-reactive solute species. We shall assume that all participating solute molecules which encounter a reactive cross-section are processed by the chemical reactions.

To model the diffusion, advective transport, and chemical reactions of the solute particles under these assumptions the following conservation equations are used for the concentrations of the solute species:

$$\frac{\partial c_A(x, y, z, t)}{\partial t} = -\nabla \cdot \mathbf{j}_A(x, y, z, t) - (-\mathbf{j}_A(0^+, y, z, t) \cdot \mathbf{e}_1) \delta(x) + (2\mathbf{j}_B(L^-, y, z, t) \cdot \mathbf{e}_1) \delta(x - L) \quad (3.1)$$

$$\frac{\partial c_B(x, y, z, t)}{\partial t} = -\nabla \cdot \mathbf{j}_B(x, y, z, t) + \left(-\frac{1}{2}\mathbf{j}_A(0^+, y, z, t) \cdot \mathbf{e}_1\right) \delta(x) - (\mathbf{j}_B(L^-, y, z, t) \cdot \mathbf{e}_1) \delta(x - L) \quad (3.2)$$

where  $c_A(x, y, z, t)$  is the concentration of solute particles of species  $A$  at location  $(x, y, z)$  at time  $t$ , and similarly for  $c_B$ . The notation  $\mathbf{e}_1$  denotes the unit vector in the  $x$ -direction. The terms  $\mathbf{j}_A$ ,  $\mathbf{j}_B$  model the fluxes of the solute species associated with the diffusion of particles, the conservative forces acting on particles, and the advective transport of particles with the fluid flow:

$$\mathbf{j}_A(x, y, z, t) = -D_A \nabla c_A(x, y, z, t) - \frac{1}{\gamma_A} \nabla V_A(x, y, z) c_A(x, y, z, t) + \mathbf{u}(x, y, z, t) c_A(x, y, z, t) \quad (3.3)$$

$$\mathbf{j}_B(x, y, z, t) = -D_B \nabla c_B(x, y, z, t) - \frac{1}{\gamma_B} \nabla V_B(x, y, z) c_B(x, y, z, t) + \mathbf{u}(x, y, z, t) c_B(x, y, z, t). \quad (3.4)$$

The first term in each of the fluxes models the diffusion of the solute by Fick's law with diffusion coefficients  $D_A$  and  $D_B$  [10,22]. The second term accounts for the conservative forces corresponding to the potentials  $V_A$  and  $V_B$  which act respectively on the solute particles of species  $A$  and  $B$ . The factors  $\gamma_A$  and  $\gamma_B$  are the drag coefficients of the solute particles of species  $A$  and  $B$  respectively [10,22]. The diffusion coefficients are related to the drag coefficients by the Einstein relations  $D_A = k_B T / \gamma_A$  and  $D_B = k_B T / \gamma_B$ , where  $T$  is the temperature in Kelvin and  $k_B$  is Boltzmann's constant [10,22]. The transport of the solute by the fluid flow is taken into account through the third term, where  $\mathbf{u}(x, y, z, t)$  is the fluid velocity at location  $(x, y, z)$  at time  $t$ . This velocity will

be derived ultimately from the osmotically induced fluid flow in a self-consistent manner with the concentration fields of the solute.

The terms involving the Dirac  $\delta$ -function [28] model the exchanges between the solute species that arise from the chemical reactions at the boundary (sources/sinks). For example, the term

$$-(-\mathbf{j}_A(0^+, y, z, t) \cdot \mathbf{e}_1) \delta(x) \quad (3.5)$$

in Eq. (3.1) models a sink for the solute flux into the cross-section corresponding to  $x = 0$ . The flux of solute coming from the right into this cross-section is given by  $-\mathbf{j}_A(0^+, y, z, t)$ . The notation  $0^+$  indicates that the value of the flux to be used is the one obtained by considering the limit of  $-\mathbf{j}_A(x, y, z, t)$  taken from the right,  $x > 0$ ,  $x \rightarrow 0$ . We remark there is no flux of  $A$  from the left of  $x = 0$  because that region is inaccessible to  $A$ , all of which is converted to  $B$  at  $x = 0$ .

In the cross-section corresponding to  $x = 0$ , the chemical reactions bind to form pairs of solute particles of species  $A$  to form solute particles of species  $B$ . The newly formed solute particles of species  $B$  are accounted for in Eq. (3.2) by the term

$$-\frac{1}{2} (\mathbf{j}_A(0^+, y, z, t) \cdot \mathbf{e}_1) \delta(x)$$

which acts as a source ejecting a concentration of  $B$  particles at the rate  $-\frac{1}{2}\mathbf{j}_A(0^+, y, z, t)$ . The factor of  $\frac{1}{2}$  arises from the stoichiometry of the chemical reaction in which two solute particles of species  $A$  form a single particle of species  $B$ .

A similar interpretation holds for the other terms involving the  $\delta$ -function. These terms model the chemical reactions which split solute particles of species  $B$ , which occur in the cross-section corresponding to  $x = L$ . The notation  $L^-$  denotes that the leftward limit  $x < L$ ,  $x \rightarrow L$  is to be taken in determining the value of the flux. The region to the right of  $x = L$  is inaccessible to  $B$ .

From the assumption that all participating solute molecules which encounter a reactive cross-section are processed by the chemical reactions, there are two additional boundary conditions:

$$c_A(0, y, z) = 0 \quad (3.6)$$

$$c_B(L, y, z) = 0. \quad (3.7)$$

We remark that non-reactive solute species are permitted in the model to freely permeate the cross-sections of the tube at  $x = 0$  and  $x = L$ . For a schematic representation of the boundary conditions see Figs. 3.1 and 2.1.

In the model the chemical reactions act either to bind together two elementary chemical units to form a molecule of species  $B$  or to separate the paired units to form two molecules of species  $A$ . Thus the elementary units are recycled in the chemical reactions and none are created or destroyed. The conservation of the total number of units throughout the chemical reactions can be expressed as:

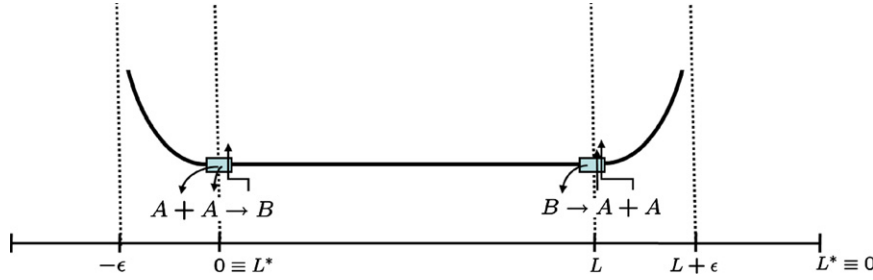
$$\int_{\mathcal{V}} (c_A(\mathbf{x}) + 2c_B(\mathbf{x})) \, d\mathbf{x} = N_0 \quad (3.8)$$

where  $\mathcal{V}$  denotes the region corresponding to the tube and  $N_0$  denotes the total number of elementary chemical units. The Eqs. (3.1) and (3.2) together with the conditions (3.6)–(3.8) give a theoretical model for the pump.

To obtain a tractable system of equations which can be solved analytically we shall reduce the model to one spatial dimension by averaging over the cross-sections of the tube (i.e., over  $y$  and  $z$ ) and thus obtaining a system of equations for the averaged concentrations as functions of the single variable  $x$ . Let the average concentration over a cross-section be denoted by:

$$C_A(x) = \frac{1}{\pi R^2} \int_{y^2+z^2 < R^2} c_A(x, y, z) \, dydz \quad (3.9)$$

$$C_B(x) = \frac{1}{\pi R^2} \int_{y^2+z^2 < R^2} c_B(x, y, z) \, dydz. \quad (3.10)$$



**Fig. 3.1.** Schematic of the potential energy. The osmotic pump is embedded in a long tube of length  $L^*$  which connects with itself to re-circulate the solvent fluid, this corresponds to periodic boundary conditions on the domain  $[0, L^*]$ . In the embedding the interior of the pump extends from  $[0, L]$ . The potential energy for the confining force is assumed to be non-zero only in a boundary layer of width  $\epsilon$  at the capping ends of the tube. A notable feature of the potential is that it is zero at the location of the reaction sites (denoted by boxes) which are modeled by appropriate source and sink terms in Eqs. (3.1) and (3.2). This prevents the confining forces from interfering with the diffusion of solute to these sites. The potential is also assumed to diverge in the boundary layer to prevent solute from diffusing outside the extended tube. We further remark that since all of solute  $A$  is converted to  $B$  at  $x = 0$ , solute  $A$  does not enter the region  $x < 0$ , so only the potential  $V_B$  is needed there to confine solute  $B$  to the tube. Similarly, all of solute  $B$  is converted to  $A$  at  $x = L$ , so only the potential  $V_A$  is needed for  $x > L$  to confine the solute  $A$ .

We also define the average flux of concentration over a cross-section by:

$$J_A(x, t) = \frac{1}{\pi R^2} \int_{y^2+z^2 < R^2} \mathbf{j}_A(x, y, z) \cdot \mathbf{e}_1 dydz \quad (3.11)$$

$$J_B(x, t) = \frac{1}{\pi R^2} \int_{y^2+z^2 < R^2} \mathbf{j}_B(x, y, z) \cdot \mathbf{e}_1 dydz \quad (3.12)$$

and the average fluid velocity by:

$$\bar{u}_0(t) = \frac{1}{\pi R^2} \int_{y^2+z^2 < R^2} \mathbf{u}(x, y, z, t) \cdot \mathbf{e}_1 dydz. \quad (3.13)$$

In this notation,  $\mathbf{e}_1$  denotes the unit vector in the axial direction ( $x$ -direction) and  $R$  is the radius of the tube. We remark that from the incompressibility of the fluid flow and the impermeability of the walls to the fluid, the flow is confined to the interior of the tube and is volume conserving, therefore, the average fluid velocity over a cross-section is independent of  $x$ .

To obtain a closed system of conservation equations for the cross-sectional concentrations we shall make a number of assumptions and approximations. For the confinement potential for the curved cylindrical boundary of the tube we take the limit of the confinement potential to a hard-wall potential,  $\xi \rightarrow 0$ . In this limit the solute can be handled by no-flux boundary conditions  $\mathbf{j}_A(x, y, z, t) \cdot \mathbf{n}_R = \mathbf{j}_B(x, y, z, t) \cdot \mathbf{n}_R = 0$  when  $y^2 + z^2 = R^2$ , where  $\mathbf{n}_R$  is the outward normal in the radial direction. Under this simplification the potentials  $V_A$  and  $V_B$  appearing in the conservation equations will be used to model only the confinement forces of the solute at the planar boundaries of the tube where the fluid can permeate. We shall also assume that the confinement forces act only in the axial direction at the ends of the tube, and require that  $V_A(x, y, z) = V_A(x)$  and  $V_B(x, y, z) = V_B(x)$ .

To obtain an expression for  $J_A$ , and similarly for  $J_B$ , we shall approximate the cross-sectional average of the term  $\mathbf{u}(x, y, z)c_A(x, y, z, t)$ , appearing when (3.3) is substituted into (3.11), by the term  $\bar{u}(t)c_A(x, t)$ . There are two different circumstances in which this would be an especially good approximation. The first is when the tube is sufficiently narrow that  $c_A(x, y, z, t)$  is effectively independent of  $y$  or  $z$ . The second is when the interior of the tube is a porous medium in which case there is a plug flow with a flat velocity profile across a section of the tube so that  $\mathbf{u}(x, y, z, t)$  is effectively independent of  $y$  and  $z$ . In both cases, the vector value  $\mathbf{u}$  would have a non-negligible component only in the  $\mathbf{e}_1$  direction since the fluid is incompressible and the tube is straight. A similar set of approximations will also be made for  $J_B$ .

With these considerations Eqs. (3.1)–(3.4) can be reduced to the conservation equations:

$$\frac{\partial C_A(x, t)}{\partial t} = -\frac{\partial}{\partial x} J_A(x, t) + J_A(x, t)\delta(x) + 2J_B(x, t)\delta(x-L) \quad (3.14)$$

$$\frac{\partial C_B(x, t)}{\partial t} = -\frac{\partial}{\partial x} J_B(x, t) - \frac{1}{2} J_A(x, t)\delta(x) - J_B(x, t)\delta(x-L) \quad (3.15)$$

with

$$J_A(x, t) = -D_A \frac{\partial C_A}{\partial x}(x, t) - \frac{1}{\gamma_A} V'_A(x) C_A(x, t) + \bar{u}_0(t) C_A(x, t) \quad (3.16)$$

$$J_B(x, t) = -D_B \frac{\partial C_B}{\partial x}(x, t) - \frac{1}{\gamma_B} V'_B(x) C_B(x, t) + \bar{u}_0(t) C_B(x, t) \quad (3.17)$$

where  $D_A = k_B T / \gamma_A$ ,  $D_B = k_B T / \gamma_B$ , and  $\bar{u}_0(t)$  is the average velocity. The cross-sectional average velocity of the flow  $\bar{u}_0$ , defined in (3.13), will be computed more explicitly in Section 3.1 by assuming a Poiseuille flow [29,30].

The absorbing boundary conditions (3.6), (3.7), and the conservation condition (3.8) extend naturally to the reduced equations, with  $C_A(0) = 0$ ,  $C_B(L) = 0$  and

$$\int_{\mathcal{V}} (C_A(x) + 2C_B(x)) dx = \frac{N_0}{\pi R^2} \quad (3.18)$$

where, as before,  $N_0$  denotes the total number of elementary chemical units. For a schematic of the one-dimensional model and the confining potential, see Fig. 3.1.

At steady-state the equations for  $C_A(x)$  and  $C_B(x)$  can be solved exactly. In Appendix A, we find the steady-state solution with the general potentials  $V_A(x)$  and  $V_B(x)$ . As mentioned above these potentials are introduced to model explicitly the solute-boundary interactions at the capping ends of the tube confining the solute and will be used mainly to model effects giving rise to osmosis. More details concerning this formulation and how osmotic effects arise will be given in Section 3.2 and Appendix B. An explicit expression for the solute concentrations can be obtained in terms of elementary functions by considering the limit in which the confining potentials at the capping ends become hard-wall potentials,  $\epsilon \rightarrow 0$ . In this limit the solute concentrations are given by (see Appendix A):

$$C_A(x) = \frac{\frac{N_0}{\pi R^2} \left[ \exp\left(\frac{\gamma_A \bar{u}_0 x}{k_B T}\right) - 1 \right]}{\left[ \frac{k_B T}{\gamma_A \bar{u}_0} \left( \exp\left(\frac{\gamma_A \bar{u}_0 L}{k_B T}\right) - 1 \right) \right] - \left[ \frac{k_B T}{\gamma_B \bar{u}_0} \left( 1 - \exp\left(-\frac{\gamma_B \bar{u}_0 L}{k_B T}\right) \right) \right]} \quad (3.19)$$

$$C_B(x) = \frac{\frac{N_0}{2\pi R^2} \left[ 1 - \exp\left(-\frac{\gamma_B \bar{u}_0}{k_B T} (L-x)\right) \right]}{\left[ \frac{k_B T}{\gamma_A \bar{u}_0} \left( \exp\left(\frac{\gamma_A \bar{u}_0 L}{k_B T}\right) - 1 \right) \right] - \left[ \frac{k_B T}{\gamma_B \bar{u}_0} \left( 1 - \exp\left(-\frac{\gamma_B \bar{u}_0 L}{k_B T}\right) \right) \right]}.$$















