



KONFERENCIA KIADVÁNY CONFERENCE PROCEEDING

Műszaki Kémiai Napok 2018
Chemical Engineering Conference 2018

2018. április 24-26.
Pannon Egyetem, Veszprém, Egyetem u. 10.

A konferencia rendezői:
Pannon Egyetem Mérnöki Kar
Biomérnöki, Membrántechnológiai és Energetika Kutatóintézete

honlapcím: <https://mkn.uni-pannon.hu>

A kiadványt összeállította és szerkesztette: Balogh András és Klein Mónika
ISBN 978-963-396-107-0

Támogatóink:



ABL&E-JASCO Magyarország Kft.
Laboratóriumi műszerek és berendezések forgalmazása

Egy nanofluidikai tranzisztor modellezése: az ionáram vezérlése a nanopórus falán lévő töltésmintázat változtatásával

Modeling of a nanofluidic transistor: controlling the ionic current with the charge pattern on the nanopore's wall

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Összefoglaló

A nanofluidikai és a mikrofluidikai eszközök közötti alapvető eltérés az, hogy a nanofluidikai eszközök esetében az elektrolitra jellemző Debye-féle árnyékolási hossz összemérhető a pórus sugarával. Ezért ezek a nanofluidikai eszközök jól alkalmazhatóak szenzorokként, diódákként, tranzisztorokként vagy éppen kapcsolókként, amelyek már nanofluidikai áramkörökbe is integrálhatóak. Egy ilyen tranzisztornál a nanopóruson átfolyó áramot a pórus falára felvitt töltések által létrehozott elektromos térrel lehet szabályozni. Ezt az elektromos teret többféleképpen hozhatjuk létre, például rögzített töltésekkel a pórus falán, amelyeket később a pH változtatásával kontrollálhatunk, vagy éppen elektródokon létrehozott polarizált töltésekkel. Így többféle nanofluidikai tranzisztort különböztethetünk meg aszerint, hogy milyen töltésekkel hoztuk létre az elektromos teret. Munkánk során két különböző elméleti módszerrel vizsgáltuk a nanopórusból létrehozható tranzisztort: egy számítógépes szimulációval (a Lokális Egyensúlyi Monte Carlo (LEMC) módszerrel) és egy átlagtér elmélettel (a Poisson-Nernst-Planck elmélettel). A két módszer a koncentrácioprofil és az elektrokémiai potenciálprofil közötti kapcsolatot különbözően teremti meg, viszont a nanopóruson átfolyó ionáramot már mindkét módszer a Nernst-Planck egyenlettel számolja. Így az NP+LEMC módszer lehetővé teszi az ionkorrelációk számítását, míg a PNP gyorsasága miatt nagyobb méretű rendszerek vizsgálatát is lehetővé teszi. A két módszer együttes alkalmazása lehetővé teszi azok előnyeinek szinergikus kihasználását.

Summary

The basic difference between nanofluidic and microfluidic devices is that in the case of nanofluidic devices the Debye-screening length is in the same range as the radius of the pore. Therefore, these devices can be used as sensors, diodes, transistors and switches which can be integrated in nanofluidic circuits. By transistor we mean that the current flowing through the nanopore can be regulated by controlling the electric field inside the pore. This electric field is produced by fixed surface charges on the wall of the nanopore and can be regulated by different chemical methods (pH, for example) or it can be polarization charges such as those induced on electrodes. Thus, nanofluidic transistors can be distinguished on the basis of the nature of charges by the kind of the electric field inside the pore is adjusted.

In this work, we present a modeling study of a nanopore-based transistor using a computer simulation method (Local Equilibrium Monte Carlo (LEMC) method) and a continuum theory (Poisson-Nernst-Planck (PNP) theory). Both methods give a solution to obtain a relation between the concentration profile and the electrochemical potential profile. After this, the current is calculated by the Nernst-Planck (NP) equation in both cases. With the NP+LEMC method it is possible to study the ionic correlations, while the PNP theory can be used for systems with larger sizes because of its fastness. Using both methods together in a multiscale modelling technique makes it possible to harvest their advantages in a synergistic way.

Modeling of a nanofluidic transistor: controlling the ionic current with the charge pattern on the nanopore's wall

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Introduction

In nanofluidic transistors the current flowing through the nanopore is regulated by controlling the electric field inside the pore. This electric field is produced by fixed charges on the nanopore's wall. There are three regions inside the nanopore due to its charge: two regions on the sides of the nanopore determine the main charge carrier ion while the task of the central region is to regulate the flow of ions with its adjustable surface charge. We present a modeling study to analyze the device behaviour to the various model parameters: surface charge density, length of the central region, dimensions of the nanopore and the concentration of the electrolyte.

Methods

In this work we present two different methods with different resolutions but the common part is the **Nernst-Planck equation**.

Ionic flux is computed:

$$-kT\mathbf{j}_i(\mathbf{r}) = D_i(\mathbf{r})c_i(\mathbf{r})\nabla\mu_i(\mathbf{r})$$

$\mathbf{j}_i$ is the flux density of ionic species, k is the Boltzmann's constant, T is temperature, $c_i(\mathbf{r})$ is the concentration profile, $\mu_i(\mathbf{r})$ is the electrochemical potential profile.

NP + LEMC method

The relation between $c_i(\mathbf{r})$ and $\mu_i(\mathbf{r})$ is established with Local Equilibrium Monte Carlo (LEMC) simulation.

$$\mu_i[n] \xrightarrow{\text{LEMC}} c_i[n] \rightarrow \mu_i[n+1]$$

The whole system is solved in an iterative way until the conservation of mass is satisfied.

Poisson-Nernst-Planck theory

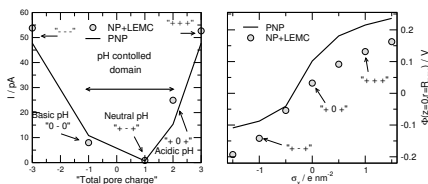
The correlation between $c_i(\mathbf{r})$ and $\mu_i(\mathbf{r})$ is established through solving the Poisson equation presuming a Boltzmann-distribution.

$$-\nabla \cdot (\varepsilon \nabla \Phi(\mathbf{r})) = \frac{1}{\epsilon_0} \sum_i q_i c_i(\mathbf{r})$$

$$c_i(\mathbf{r}) = c_i^0 \exp(-q_i \Phi(\mathbf{r})/kT)$$

Conclusion

1. Experimentally the surface charges are provided by protonated and deprotonated chemical groups, thus pH is a tool to tune the electric field. In this work, effect of the surface charge can correspond to the effect of the pH and potential.



2. In our case, small dimensions and large surface charge allow local effects in addition to long-range effects of applied field, which is an advantage of nanodevices over microdevices.

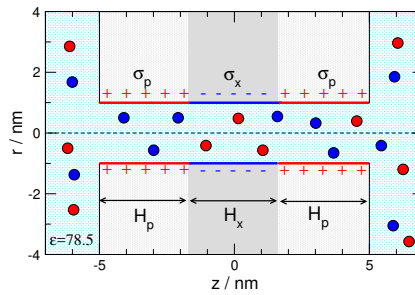
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Acknowledgements

This work was supported by the Hungarian National Research, Development and Innovation Office (NKFIH K124353), Project No. GINOP-2.3.2-15-2016-00053 and UNKP-17-4. (M.V.)

Model



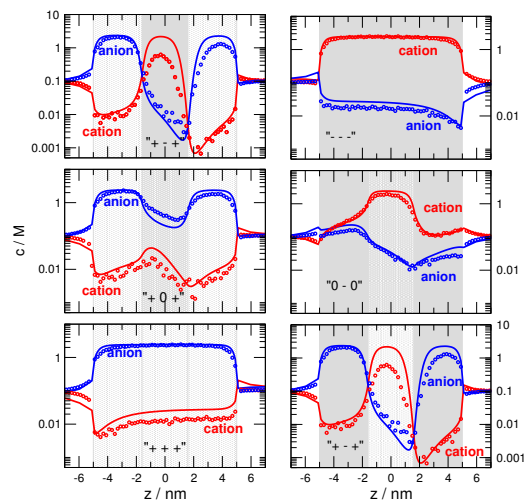
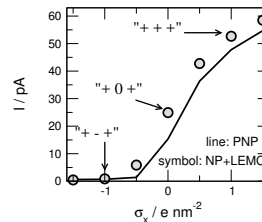
Schematics of the cylindrical nanopore that has three regions of lengths (H_p , H_x and H_p) with charge densities (σ_p , σ_x and σ_p).

- Nanopore is cylindrical pore penetrating a membrane, $H_{\text{pore}} = 10$ nm and $R_{\text{pore}} = 1$ nm
- Hard walls for both the membrane and the pore
- Primitive Model of electrolytes is used for the ions (charged hard spheres) in the case of NP+LEMC, in PNP the ions are modelled as point charges
- Surface charge: Neumann boundary conditions in PNP, fixed point charges in NP + LEMC
- The electrolyte inside the pore and on the two sides of the membrane is represented as charged hard sphere ions immersed in a dielectric continuum of dielectric constant $\epsilon = 78.5$.

Results

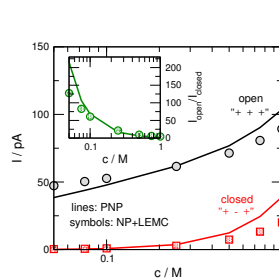
Effect of the charge pattern: changing surface charges

- Value of σ_p defines the main charge carrier ion and the value of σ_x tunes the depletion zones for it
- The current is controlled by the depth of the depletion zone of the charge-carrying ion in the region whose charge density is controlled
- The device function ($I_{\text{open}}/I_{\text{closed}}$) shows the usefulness of the transistor as a switch



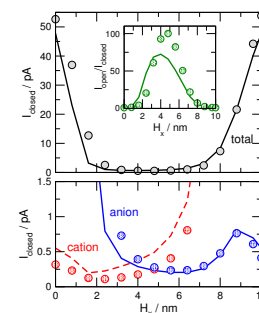
Effect of the concentration

- Both currents in open and closed state increase with the increasing concentration
- Although the $I_{\text{open}}/I_{\text{closed}}$ ratio is higher in smaller concentrations



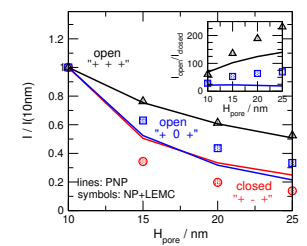
Effect of the length of the central region: changing region widths

- Fixed charge densities and changing the widths of H_x and H_p , while the H_{pore} is fixed for 10 nm
- Reason of the extremum: both regions have sufficient size to produce sufficiently deep depletion zones



Effect of the length of the nanopore

- The absolute value of the current is smaller for longer pores due to deeper depletion zones
- Currents decrease faster in the closed state than the open states, consequence: device function improves



Effect of the pore radius

- Debye screening length (λ_D) characterizes the thickness of the double layer
- Increasing pore radius inhibits the formation of depletion zones because of the smaller overlapping of the double layers
- Device behaviour scales with the $R_{\text{pore}}/\lambda_D$

