# 3

## Selective electrodifussion in nanochannels

## Katarzyna Tkacz-Śmiech<sup>\*</sup>, Bogusław Bożek, Marek Danielewski

AGH - University of Science and Technology, Al. Mickiewicza 30, 30-059 Kraków, Poland  $^{*} \rm Corresponding \ author$ 

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## Introduction

Bio - mimetic materials represent a class of synthetic architectures designed from knowledge of biology. However, nature is still far ahead of technology and therefore there is a big interest in understanding the generic phenomena and processes occurring in living organisms. In recent years intensive research has started to examine and describe the functions of channel proteins in the living eucaryota and procaryota cell membranes [1-4]. They separate cell interior and exterior, can fluctuate between open and closed states and mediate the transport of specific inorganic ions, primarily Na<sup>+</sup>, K<sup>+</sup>, Ca<sup>2+</sup> cations and Cl<sup>-</sup>anions. Due to an ability of these channels to control ionic transport they are referred to as ion channels. In open state, they work as selective filters, permitting some ions to pass, but limiting the rate of passing of the others. The transported ions diffuse downhill the gradient of electrochemical potential, without coupling to an energy source (metabolic energy, like ATP).

The cell channels open in response to specific stimulus, like: change of the voltage across the membrane, mechanical stress or binding ligands. Most interesting is however the ability of the channels to work as selective filters in the open conformation. Just this ability is a key for considering the ion channels as "nano-smart-machines" witch are essential for many cell functions, including excitability of muscle cells or conduction of electrical signaling in nervous system.

Unfortunately, although more than 1000 types of ionic channels have been described with new ones constantly being discovered, the understanding of the selectivity mechanism in molecular channels in still lacking and the studies in this area cover extensively developed research activity at the intersection of electrochemistry and nanotechnology [5-9]. It is believed that learning and understanding of the selective transport of ions through the channels will give rise towards real-world applications and will provide guidelines to design and fabricate synthetic nanopores to be applied in sensing, purifying or energy conversion [10-11].

## Modeling of the transport properties of ion channels

The approaches that give conceptualization of the ionic transport across the molecular channel include kinetic and stochastic models (MD - molecular dynamics and BD - Brownian dynamics, respectively) and continuum models covering Poisson - Boltzmann (PB) and Nernst - Planck - Poisson (NPP) theories [5-9,12,13]. It is however not our intention to review here all these approaches. We aim to argue that the transportive properties of IC can be explored as arising from the average transport properties of electrodiffusion as stated in NPP method. Therefore, we present only very brief description of the other three approaches.

#### Molecular and Brownian dynamics

In molecular dynamics (MD), the trajectories of N particles are simulated from Newton's motion equations [14]. The interactions between moving particles, water and amino acid functional groups are usually described by utilizing empirical potentials or force fields, like Coulomb or Lennard Jones functions calibrated by macroscopic data. Application of MD to simulate the transport of many ions in the molecular channel is limited by two issues: (i) a proper choice of the field, (ii) computational costs [7,8,14,15].

The computational difficulties are partially eliminated in Brownian dynamics (BD) method in which only chosen interactions are considered. It is in particular assumed in BD that the net force acting on the particle can be represented as a sum of friction force and white noise with a zero mean. In this case, Newton equations can be replaced by Langevin stochastic equations [16,17].

#### Poisson - Boltzmann and Nernst - Planck - Poisson models

In continuum models, the computational costs are reduced by using an approximation of continuous media. Poisson - Boltzmann (PB) theory predicts that the set of ions can be described using the charge density function represented by the Boltzmann type factor dependent upon averaged electric potential calculated from Poisson equation. Combing of Boltzmann expression for ion density with Poisson equation leads to PB equations which can be easily solved [18,19].

Nernst - Planck - Poisson (NPP) theory involves elecrodiffusion in which transported species are treated as charge densities of continuous distributions and they are calculated from NPP equations [20-29]. Consequently, both PB and NPP theories neglect the possible effects due to different ionic volumes. The other limitation concerns neglecting of non - electrostatic interactions between the ions.

NPP theory has been successfully applied to model the transport of ions in liquids and semiconductors. Various numerical algorithms were used to solve NPP equations including: finite difference, finite element and finite volume methods [4,26,28,29].

## Downhill electrodiffusion of ions in the channel. General formulation

The so called potassium channels, permeable mostly for potassium cations, conduct  $K^+$  10000 fold better than smaller Na<sup>+</sup> cations (the radiuses of the cations are 0.133 nm and 0.095 nm for  $K^+$  and Na<sup>+</sup>, respectively). Therefore, it is obvious that the normal selectivity of the channels in their open conformation cannot be explained by pore size and it is believed that it can be explained with reference to eletrodiffusion principles [26,28-30].

In this section we present a mathematical conceptualization of transportive properties of molecular channel based on electrodiffusion principles. We assume that the channel is an open cylinder which connects two baths with the ions (left -L and right -R). The baths are large and relatively small amounts of transferred ions do not change the ionic concentrations in the reservoirs. The present model includes:

- tri- dimensionality of the channel,
- external electrostatic potential applied to channel walls in two different ways (locally at two rings or linearly increasing over the entire length), Fig. 3.1.

Tri-dimensionality allows for future considering complex shapes of the channel, like cavity or necking, and therefore it seems more convenient. Thanks to introducing the external potential a presence of charged amino acids at the channel walls can be mimicked as well. Besides we assume what follows:

(i) each ionic species is treated as continuous fluid of the concentration which is a function of time and position  $c_i = c_i(x, t)$ ;

- (ii) the movement of ions perpendicular to the channel axis is allowed (3D problem);
- the downhill ionic transport is driven by concentration gradient and electric field (Nernst - Planck flux);
- (iv) electric field acting on the ions comes from the external potential and electrostatic self consistent potential induced by electric charges of the ions in the channel (Poisson equation);
- (v) the concentrations of the ions in the channel can be calculated from the 3D mean field NPP equations;
- (vi) the ions are not allowed to escape thorough the channel walls.



A scheme of a channel connecting two reservoirs of ions: a) channel geometry, b) a way of potential application. The segments  $\partial \Omega_{1-7}$  and  $\partial \Omega^*$  are indicated

The general equations that govern the electrodiffusion of ions in the channel are:

1) Nernst - Planck equation, which determines the flux  $J_i = J_i(x,t)$  of the *i*-th specie (i = 1, ..., N) of the charge  $z_i$  and self-diffusivity  $D_i$ :

$$J_i = -D_i \left( \nabla c_i - z_i \gamma c_i E \right), \quad i = 1, \dots, N ,$$
<sup>(1)</sup>

where  $\gamma = \frac{F}{RT}$  is a temperature dependent constant, where F and R are Faraday and gas constants.

The above equation governs a specie's movement driven by electric field, E, and concentration gradient  $\nabla c_i$ . The first term in it represents Fickian diffusion flux and the second one accounts for the interaction with the electric field.

Generally the fluxes of the ions are considered as electrodiffusion fluxes and drift is ignored (convection,  $J_i^{drift} = c_i v^{drift} \approx 0$ ). It is more prospective however to include both terms and consider the total (diffusion plus drift) flux [4,26,28]:

$$\tilde{J}_i = J_i + J_i^{drift};$$
<sup>(2)</sup>

2) The concentrations of the ions and the electric field are coupled through Poisson equation:

$$\nabla \cdot E = \frac{\rho}{\varepsilon} \,. \tag{3}$$

In the above,  $\varepsilon$  is dielectric constant of the medium and  $\rho$  is a total time- and position dependent charge density, calculated as the sum of the densities of all ions:

$$\rho = \rho(x,t) = \sum_{i=1}^{N} \rho_i = F \sum_{i=1}^{N} z_i c_i .$$
(4)

Equations (1) - (3) are known as NPP equations. They are coupled, i.e. the flux  $J_i$  moves the charge  $\rho_i$  and thereby changes the electric field E and the concentration  $c_i$ . Mathematically it means that the concentrations,  $c_i$  (i = 1, ..., N), allow determining the total charge,  $\rho = \rho(x, t, c_i (\tilde{x}, t)_{i=1,...,N})$ , and the electric field  $E = E(x, t, c_i (\tilde{x}, t)_{i=1,...,N})$ . Hence the concentrations  $c_i$  (i = 1, ..., N) can be calculated using Nernst- Planck equations, Fig. 3.2.



#### FIGURE 3.2

Coupling between Nernst – Planck and Poisson equations

The mass conservation requires a continuity equation to be satisfied:

$$\frac{\partial c_i}{\partial t} + \nabla \cdot \tilde{J}_i = 0.$$
<sup>(5)</sup>

In the above sources and/or sinks are neglected. At the stationary state the flux is independent of time and position, and:

 $\nabla \cdot \tilde{J}_i = 0 . ag{6}$ 

Combining above we get:

$$\frac{\partial c_i}{\partial t} = D_i \left( \nabla^2 c_i + \gamma z_i \nabla c_i \cdot \nabla \varphi + \gamma z_i c_i \nabla^2 \varphi \right) - \nabla \cdot \left( c_i v^{drift} \right) \text{ for } i = 1, \dots, N ,$$
(7)

where 
$$\nabla^2 \varphi = -\frac{F}{\varepsilon} \sum_{i=1}^N z_i c_i$$
.

For the channel of cylindrical symmetry the above problem can be transformed into cylindrical coordinates (x, r) in  $\mathbb{R}^3$ :

$$\frac{\partial c_i}{\partial t} = D_i \left( \frac{\partial^2 c_i}{\partial x^2} + \frac{\partial^2 c_i}{\partial r^2} + \frac{1}{r} \frac{\partial c_i}{\partial r} + \gamma z_i \left( \frac{\partial c_i}{\partial r} \frac{\partial \varphi}{\partial r} + \frac{\partial c_i}{\partial x} \frac{\partial \varphi}{\partial x} \right) + \gamma z_i c_i \left( \frac{\partial^2 \varphi}{\partial x^2} + \frac{\partial^2 \varphi}{\partial r^2} + \frac{1}{r} \frac{\partial \varphi}{\partial r} \right) \right)$$
(8)

for i = 1, ..., N and neglected drift  $v^{drift} = 0$ , and where:  $\frac{\partial^2 \varphi}{\partial x^2} + \frac{\partial^2 \varphi}{\partial r^2} + \frac{1}{r} \frac{\partial \varphi}{\partial r} = -\frac{\rho}{\epsilon} = -\frac{F}{\epsilon} \sum_{i=1}^{N} z_i c_i$ .

### Simulations

The present simulations were made for the following case:

- (i) the channel is a cylinder of a length L and radius R, such that  $(x,r) \in [0,L] \times [0,R]$ ;
- (ii) the external potential is applied to the channel walls, either at two rings or along the cylinder side as the potential varying linearly, Fig. 3.1;
- (iii) a medium inside the channel is water of the temperature 310 K;
- (iv) the baths contain KCl and NaCl solutions at given concentrations, thus  $K^+$ ,  $N^+$  and  $Cl^-$  ions are transported through the channel: N = 3 and  $i = K^+$ ,  $Na^+$ ,  $Cl^-$ .

#### **Boundary conditions**

Due to cylindrical symmetry of the channel, the Neuman boundary conditions are put at the rotation axis:

$$\frac{\partial c_i}{\partial r} = 0 \quad \text{for } r = 0 \;. \tag{9}$$

The other boundary conditions are defined on a domain  $\partial \Omega = \bigcup_{k=1}^{7} \partial \Omega_i$  - for the channel provided with the rings and  $\partial \Omega = \bigcup_{k=1}^{2} \partial \Omega_i \cup \partial \Omega_{\varphi}$  - for the channel subjected to the potential linearly increasing along the channel side. The segments  $\partial \Omega_1$  and  $\partial \Omega_2$  are open ends connected to the left (L) and right (R) reservoirs. They are permeable and let the ions enter/exit the channel. The concentrations at  $\partial \Omega_1$  and  $\partial \Omega_2$  are the same as the concentrations in the baths:

$$c_i(\mathbf{x},t) = c_i^L(\mathbf{x},r) = \text{const}_1 \text{ for } \mathbf{x} \in \partial \Omega_1,$$
  

$$c_i(\mathbf{x},t) = c_i^R(\mathbf{x},r) = \text{const}_1 \text{ for } \mathbf{x} \in \partial \Omega, \text{ and } i = K^+, Na^+, CI^-$$

The ions cannot leave the channel through the walls ( $\partial \Omega_{3-7}$  and  $\partial \Omega_{\varphi}$ ) and zero-flux boundary condition is put at these fragments:

$$J_{i}(\mathbf{x},t) = 0 \quad \text{for } \mathbf{x} \in \partial \Omega_{3-7} \text{ and } \mathbf{x} \in \partial \Omega_{\varphi},$$
(10) which is equivalent to:

$$\frac{\partial c_i}{\partial r} + \gamma z_i c_i \frac{\partial \varphi}{\partial r} = 0.$$
(11)

Besides, the boundary conditions for the potential are established:

$$\frac{\partial \varphi}{\partial r}(\mathbf{x},t) = 0 \quad \text{at} \quad \mathbf{x} \in \partial \Omega_{3,5,7} \tag{12}$$

and

$$\varphi(\mathbf{x}) = \varphi_L(\mathbf{x},t) = \varphi_L$$
 at  $\mathbf{x} \in \partial \Omega_4$ ,  $\varphi(\mathbf{x}) = \varphi_R(\mathbf{x},t) = \varphi_R$  at  $\mathbf{x} \in \partial \Omega_6$ ;  $\varphi_L - \varphi_R = \Delta \varphi$ 

or

$$\varphi\left(\mathbf{x}\right)=\varphi\left(\mathbf{x},t\right)=\tilde{\varphi}\left(\mathbf{x}\right),\text{ at }\mathbf{x}\in\partial\Omega_{\varphi}\text{,}$$

where  $\tilde{\phi}(x)$  given by a linear dependence such that:

 $\tilde{\varphi}(x=0) - \tilde{\varphi}(x=L) = \tilde{\varphi}_L - \tilde{\varphi}_R = \Delta \tilde{\varphi} \,.$ 

The system of Eqs. (8) - (11) was solved for the above boundary conditions using Crank-Nicolson difference scheme.

#### Data

To examine transport properties of cylindrical channel with external electric potential applied to the walls the series of numerical experiments have been made, in which we have calculated:

- the concentrations of the ions,
- electrostatic potential,
- fluxes and flows of the ions,
- charge distribution and the current.

The program allows presenting the results as 2D maps and 3D graphs at the central cross section but only chosen figures are shown here.

The data used in simulations are summarized in Tables 3.1-3.2, 3.4-3.6 and the scheme of the performed numerical experiments is shown in Fig. 3.3.

For further convenience, we will be using in the following the symbols A-C to distinguish various compositions, preceded by either "1" or "2" for various ways of application of the potential, as defined in the last row of Table 3.1.

The time evolution and the effects of the channel dimensions, applied voltage and potential distribution (green color in Fig. 3.3) are studied for one chosen set of data (Experiment 1B for the linearly varying potential), Figs. 3.4, 3.11. For other experiments (grey color) we present the concentration, charge density and potential distributions in the channel at the stationary state (Figs. 3.5-3.10).

#### TABLE 3.1

The constant parameters used in simulations of the ionic transport in the channel

|  | lons                  |                       | Medium: water  |
|--|-----------------------|-----------------------|--|
| K <sup>+</sup> Na <sup>+</sup> Cl <sup>-</sup> |                       |                       | Temperature: 310 K   |
|  | Diffisivity [m²/s]    | ]                     | Dielectric constant $\varepsilon_w$ =80 $\varepsilon_0$ =708,335×10 <sup>-12</sup> F/m |
| 2.2·10 <sup>-9</sup>                           | 1.33·10 <sup>-9</sup> | 2.03·10 <sup>-9</sup> | $\gamma = \frac{F}{RT} = 37.44 \text{ C/J}$  |

#### TABLE 3.2

The data used in the simulations

|      | Concentrations [mol/m <sup>3</sup> ] |         |     |             |                                     |     | Channel dimensions                         |      |                  |                  |                    |                          |
|------|--------------------------------------|---------|-----|-------------|-------------------------------------|-----|--|------|------------------|------------------|--------------------|--------------------------|
| E.v. |                                      |         |     |             |                                     |     | Length <i>, L</i> [nm]                     |      |                  | R                | Radius, R [nm]     |                          |
| EX.  | X. Loft both Dight both              |         |     |             | ۰h                                  | 10  |  |      |                  | 5                |                    |                          |
|      | L                                    | en bai  | 11  | Kigiit bath |                                     |     | Potential                                  |      |                  |                  |                    |                          |
|      | lons lons                            |         |     |             | 1. at the rings 2. varying linearly |     |  |      |                  | nearly           |                    |                          |
|      | Na⁺                                  | $K^{+}$ | Cl  | Na⁺         | $K^{+}$                             | Cl  | $\varphi_L \qquad \varphi_R \qquad \Delta$ |      | $\Delta \varphi$ | $	ilde{arphi}_L$ | $	ilde{arphi}_{R}$ | $\Delta \tilde{\varphi}$ |
| А    | 250                                  | 250     | 500 | 25          | 25                                  | 50  | [mV]                                       | [mV] | [mV]             | [mV]             | [mV]               | [mV]                     |
| В    | 250                                  | 25      | 275 | 25          | 250                                 | 275 | 20   | 10   | 20               | 20               | 10                 | 20                       |
| С    | 250                                  | 25      | 275 | 250         | 25                                  | 275 | 20   | -10  | 30               | 20               | -10                | 30                       |
| Expe | Experiments: 1A, 1B, 1C, 2A, 2B, 2C  |         |     |             |                                     |     |  |      |                  |                  |                    |                          |



#### FIGURE 3.3

Scheme of the performed numerical experiments. In green numerical experiments performed entirely for the experiment 1B

### Results



The results of the calculations are presented in Figs. 3.4-3.11 and tables 3.3-3.5.

#### FIGURE 3.4

Time evolution of the total charge density in the channel in comparison with the results for the stationary state. 2D maps (first row) and 3D graph (second row).

The results for the channel with the voltage increasing linearly between -10 mV and 20 mV from the right to the left end of the channel, Experiment 1B in Table 3.2 and Fig. 3.3.

The charge density given inF/m<sup>3</sup>

In the next set of figures, Figs. 3.5-3.9 the results obtained for various concentrations of the ions in the baths are compared (Experiments 1A-C, 2A-C).

The series of the results are for different ways of application of the external potential but the same potential differences (voltages):  $\Delta \varphi$  and  $\Delta \tilde{\varphi}$ . The respective figures show: concentration of the ions, Figs. 3.5-3.7, potential, Fig. 3.8, and total charge distribution, Fig. 3.9.



2D maps of the concentration of the potassium ions in the channel, at the central cross section. The results for various concentrations of the ions in the baths, Experiments 1A-C, 2A-C. Concentrations in  $mol/m^3$ 



#### FIGURE 3.6

2D maps of the concentration of the sodium ions in the channel, at the axis intersection. The results for various concentrations of the ions in the baths, Experiments 1A-C, 2A-C. Concentrations in  $mol/m^3$ 



2D maps of the concentration of the chlorine ions in the channel, at the axis intersection. The results for various concentrations of the ions in the baths, Experiments 1A-C, 2A-C. Concentrations in  $mol/m^3$ 



#### FIGURE 3.8

2D maps of the electrostatic potential in the channel, at the axis intersection. The results for various concentrations of the ions in the baths, Experiments 1A-C, 2A-C. Potential in mV



2D maps of the total charge distribution in the channel, at the axis intersection. The results for various concentrations of the ions in the baths, Experiments 1A-C, 2A-C. The charge density inF/m $^3$ 

The results confirm a coupling between charge (ion) distribution and the potential. The potential disturbs the concentration of the ions in the channel and vice versa.

From the concentrations the fluxes have been calculated and hence the overall flows of the ions and the total flow of the charges (current) in the channel have been determined, Table 3.3.

#### TABLE 3.3

Overall flows of  $K^{+}$ ,  $Na^{+}$  and  $Cl^{-}$ ions through the channel for various concentrations in the baths, Experiments 1A-C, 2A-C

| Potential                         | F۷ | Current x 10 <sup>10</sup> | Flow x 10 <sup>15</sup> [mol/s] |      |       |  |  |
|-----------------------------------|----|----------------------------|---------------------------------|------|-------|--|--|
| Fotential                         | LA | [A]                        | Na+                             | K+   | CI-   |  |  |
| 1. varying linearly between -     | А  | 3,3                        | 3,2                             | 5,2  | 4,9   |  |  |
| right to the left end:            | В  | 3,3                        | 3,1                             | -2,5 | -2,6  |  |  |
| $\Delta \tilde{\varphi} = 30  mV$ | С  | 4,4                        | 1,6                             | 0,2  | -2,5  |  |  |
| 2 applied at the rings            | А  | -0,6                       | 2,4                             | 4    | 6,8   |  |  |
| only: $\Delta \phi = 30 mV$       | В  | -1,15                      | 2,3                             | -3,6 | -0,2  |  |  |
|                                   | С  | 0,3                        | 0,1                             | 0,02 | -0,18 |  |  |

The results confirm that the flow is constant along the channel which is an expected result for the stationary state. The calculated flows are compared in Table 3.3 and Fig. 3.10. Positive flow refers to the movement of the ions from the left to the right bath. It is clearly seen that a way of application of the potential is essential for the transportive channel properties. In particular the transport of the ions can be forced by the potential difference only, at zero concentration gradient.



Overall flows of the ions(a) and the current in the channel (b); crosses – for the linearly varying potential, spots – for the potential applied at the rings; green – sodium ions, red – potassium ions, blue – chlorine ions. The results for the experiments 1A-C, 2A-C

The potential differences (voltage) between the left and right ends of the channel are summarized in Tables 3.4-3.5 and Fig. 3.11. The presented results have been obtained for the channel with the potential linearly varying, Experiment 1B. It seen that for the same concentrations and the same voltage,  $\Delta \tilde{\varphi} = 30 mV$ , the current and ionic flows are the same, i.e. they do not depend on the boundary potentials but on their difference only, Table 3.4.

The dependencies between the flows of the ions and the voltage are presented in Table 3.5 and Fig. 3.11a. In Fig. 3.11b the current-voltage characteristics is shown. In all cases linear dependencies are observed, characteristic for ohmic-like behavior. The results confirm that application of the potential of given difference between the channel entrance and exit allows controlling both the direction and the heights of the flows of the ions.

It means that the potential is a decisive factor for the selectivity of the channel.

#### TABLE 3.4

Overall flows of  $K^*$ ,  $Na^*$  and  $Cl^-$  ions and the current in the channel subjected to the same voltages but various left and right boundary potentials. The results for the experiment 1B

| Left                    | Right                         |                            | Current x 10 <sup>10</sup> | Flow x 10 <sup>15</sup> [mol/s] |      |      |  |
|-------------------------|-------------------------------|----------------------------|----------------------------|---------------------------------|------|------|--|
| $	ilde{arphi}_{L}$ [mV] | $	ilde{arphi}_{_R}[{\sf mV}]$ | $\Delta 	ilde{arphi}$ [mV] | [A]                        | Na+                             | K+   | Cl-  |  |
| -20                     | 10                            | -30                        | 3,3                        | 3,1                             | -2,5 | -2,6 |  |
| -10                     | 20                            | -30                        | 3,3                        | 3,1                             | -2,5 | -2,6 |  |
| 0                       | 30                            | -30                        | 3,3                        | 3,1                             | -2,5 | -2,6 |  |
| 10                      | 40                            | -30                        | 3,3                        | 3,1                             | -2,5 | -2,6 |  |
| 20                      | 50                            | -30                        | 3,3                        | 3,1                             | -2,5 | -2,6 |  |
| 30                      | 60                            | -30                        | 3,3                        | 3,1                             | -2,5 | -2,6 |  |

#### Flow x $10^{15}$ [mol/s] Left Right Current x 10<sup>10</sup> $\tilde{\varphi}_{r}$ [mV] $\tilde{\varphi}_{P}[mV]$ K+ CI- $\Delta \tilde{\varphi}$ [mV] Na+ [A] -2,5 20 -10 3,3 -2,6 30 3,3 -3 10 -10 20 1,7 3 -1,8 0 -10 10 2,6 -3,4 -1 0,1 -10 -10 0 -1,48 2,2 -3,9 0 -20 -10 -10 -3,1 2 -4,4 1 -30 -10 -20 -4,8 -5 1,8 1,8 -40 -10 -30 -6,6 1,5 -5,5 2,75

#### TABLE 3.5

Overall flows of  $K^{\dagger}$ ,  $Na^{\dagger}$  and  $Cl^{-}$  ions and the current in the channel subjected to various voltages. The results for the experiment 1B

The next series of calculations have been made for the ionic channels of various dimensions. The results are summarized in Table 3.6. The data present total current and the flows of the ions. Besides average fluxes and current density, calculated as the flows/current divided by the channel cross section area are presented.

It is seen that both current density and average fluxes increase with narrowing of the channel. It is an obvious effect of the electricfield which in the narrow channel is stronger. Of course the total current/flows decrease in the narrow channel.



#### FIGURE 3.11

Flow of ions vs. voltage (a) and current voltage characteristics (1b) for the channel. The results for the experiment 1B

#### TABLE 3.6

Total current, current density, overall flows and average fluxes of the ions in the channels of various sizes. The results for the experiment 1B

|      | Longth | Radius | Current | Current             | Overa | all flow :<br>[mol/s] | x 10 <sup>15</sup> | Avera<br>[ | age flux ><br>mol/sˈm² | ( 10 <sup>33</sup><br>] |
|------|--------|--------|---------|---------------------|-------|-----------------------|--------------------|------------|------------------------|-------------------------|
| [mV] | L [nm] | r [nm] | [A]     | $x 10^{29} [A/m^2]$ | Na+   | K+                    | Cl-                | Na+        | K+                     | Cl-                     |
|      | 30     | 5      | 1,6     | 0,204               | 1,2   | -0,7                  | -1,2               | 0,015      | -0,155                 | -0,780                  |
| 30   | 20     | 5      | 2,2     | 0,280               | 1,7   | -1,1                  | -1,6               | 0,022      | -0,121                 | -0,421                  |
|      | 10     | 5      | 3,3     | 0,420               | 3,3   | -2,5                  | -2,6               | 0,042      | -0,073                 | -0,132                  |
|      | 10     | 2,5    | 1,28    | 0,652               | 0,8   | -0,5                  | -0,9               | 0,041      | -0,249                 | -1,146                  |
|      | 10     | 0,5    | 0,066   | 0,840               | 0,04  | -0,045                | -0,017             | 0,051      | -8,952                 | -2,672                  |

## Summary

Ion channels, present in biological membranes, have an important role in maintaining living cells. Despite new technologies that allow an examination of the channel structure, the fundamental functioning of this nature wonder are still not well understood, particularly the selectivity mechanism remains a mystery. New insights of the transportive properties of the channel can be revealed using numerical simulations.

In this chapter a new 3D model of the channel with the walls subjected to the external potential has been presented. The results confirm that the potential distribution is mainly responsible for the selectivity mechanism. The advantages of the model are: tri-dimensionality and possibility of including drift which seem particularly prospective as far as real biological systems are considered.

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## References

- 1. B. Alberts, A. Johnson, J. Lewis, M. Raff, K. Roberts and P. Walter, Molecular Biology of the Cell, Taylor & Francis Group, 5th Edition, 2007
- 2. D. Purves, G.J. Augustine, D. Fitzpatrick, W.C. Hall, A.-S. LaMantia and L.E. White Neuroscience. 2012, Sinauer Associates, Inc., 5th Edition, 2012
- 3. S.-H. Chung, S. Kuyucak, Biochimica et Biophysica Acta (BBA) Biomembranes 1565 (2002) 267
- 4. B. Bozek, B. Wierzba, M. Danielewski, Defect Diff. Forum 1467 (2010) 297
- 5. M. Saraniti, S. Aboud, and R. Eisenberg, Rev. Comp. Chem. 22 (1999) 229

- 6. B. Eisenberg: Channels, receptors, and transporters in Biophysics textbook on line, Chapter 4, http://www.biophysics.org/education/eisenberg.pdf
- 7. M. Tagliazucchi and I. Szleifer, Materials Today 18 (2015) 131
- 8. C. Maffeo, S. Bhattacharya, J. Yoo, D. Wells and A. Aksimentiev, *Chem. Rev.* 112 (2012), 6250
- 9. B. Cornell, V. L. Braach-Maksvytis, L. G. King, P. D. Osman, B. Raguse, L. Wieczorek, and R. J. Pace, Nature 387 (1997) 580.
- 10. C. Hélix-Nielsen, Anal. Bioanal. Chem. 395 (3) 697
- 11. K. Cammann, Working with Ion-Selective Electrodes. Chemical laboratory Practice.: Springer-Verlag Berlin Heidelberg, 1979
- 12. K. Cooper, E. Jakobsson, P. Wolynes, Prog. Biophys Molec. Biol. 46 (1985) 51
- 13. B. Corry, S. Kuyucak, S-H. Chung, Biophys. J. 78 (2000) 2364
- 14. S.-H. Chung and S. Kuyucak, Europ. Biophys. J. 31(2002): p. 283
- B. C. Bennett, M. D. Purdy, K. A. Baker, Ch. Acharya, W. W McIntire, R. C. Stevens, Q. Zhang, A. L. Harris, R. Abagyan and M. Yeager, Nature Communications 7 doi: 10.1038/ncomms9770B
- 16. Nadler, Z. Schuss, A. Singerand, R.S. Eisenberg, J. Phys.: Condens. Matter. 16 (2004) S2153
- 17. J. Miękisz, J. Gomułkiewicz and S. Miękisz, Math. Appl. 42 (2014) 39
- 18. G. Moy, B. Corry, S. Kuyucak, and S. H. Chung, Biophys. J. 78 (2000) 2349
- 19. B. Corry, S. Kuyucak, S-H. Chung, Biophys. J. 84 (2003) 3594
- 20. V. Barcilon, D.P. Chen, R.S. Eisenberg, J. Appl. Math. 52 (1992) 1405
- 21. D.P. Chen, V. Barcilon, R.S. Eisenberg, Biophys. J. 61 (1992) 1372
- 22. D. P. Chen, R. S. Eisenberg, Biophys. J. 64 (1993) 1405
- 23. D.P. Chen, J. Lear, R.S. Eisenberg, Biophys. J. 72 (1997) 97
- 24. I. Valent, P. Petrovič, P. Neogrády, I. Schreiber and M. Marek, J. Phys. Chem. B 117 (2013) 14283
- 25. R. A. Arndt, L.D. Roper, Math. Biosciences 16 (1973) 103
- 26. B. Bozek, A. Lewenstam, K. Tkacz-Śmiech and M. Danielewski, ECS Transaction 61 (2014) 11
- 27. W. Liu, J. Diff. Equ. 246, 428 (2009)
- 28. B. Bozek, H. Leszczyński, K. Tkacz-Śmiech and M. Danielewski, Defect Diff. Forum 363 (2015) 68
- 29. J.-L. Liu, B. Eisenberg, Phys. Rev. E 9 (2015) 012711
- D. A. Doyle, J.M. Cabral, R. A. Pfuetzner, A. Kuo, J. M. Gulbis, S. L. Cohen, B.T. Chait, R. MacKinnon, Science 280 (1998) 69