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Rough estimation of the coefficients in mathematical models describing ion flux through cellular membrane

Václav Čibera[1]

Introduction

Recent developments in medical and biological science have heightened the need for understanding processes on the cellular level. To the most significant processes on the cellular level belong fluxes of ions through the cellular membrane. Ion fluxes through membrane are carried out by special proteins called ion channels. Functionality of these molecular mechanisms significantly affect proper functionality of the whole cell.

Experiments still play a key role in acquiring new knowledge in this field. In addition to experiments there is another approach in acquiring new knowledge using mathematical modelling. Although many mathematical models describing ion flux through membranes were introduced in the last decades, there is still no universal suitable approach. This paper introduces two approaches for description ion flux through the ion channels: *Nernst-Planck equation* and equation based on the description using *electrochemical potential*. Some comments and rough estimations to determine the coefficients in these two equations are given.

Mathematical models describing ion flux through cellular membrane

Concentration gradient and gradient of electric field are present across the cellular membrane. Therefore mathematical models mainly consist of two parts describing these two gradients and of the coefficients. Two equations are well known besides other models for description of the considered phenomena. The first is **Ion flux described by electrochemical potential**:

$$J = \frac{1}{\Theta}\left[RT\ln\frac{c_{in}}{c_{out}} + zFU\right], \tag{1}$$

where J is the number of ions crossing a channel per second, Θ is the resistance coefficient, R is universal gas constant, T is absolute temperature, c_{in} is internal ion concentration of considered ions, c_{out} is external ion concentration, z is the valence of the ion, F is Faraday's constant, U is voltage across membrane. Besides of resistance coefficient Θ all variables or constant can be found in literature. Rough estimation of this coefficient is shown in result section.

The second expression is **Nernst-Planck electro-diffusion equation**:

$$J = -D\left(\frac{dc}{dx} + \frac{c(x)zF}{RT}\frac{d\varphi}{dx}\right), \tag{2}$$

where D is diffusion coefficient , c is the ion concentration, $x \in [0, d]$ where d is the thickness of the membrane. φ is the electric field potential. Assuming the same voltage V across ion channel one can obtain solution of (2) in the form:

$$J = -\frac{\frac{DzVF}{RTd}\left[c_{in} - c_{out}\exp(-\frac{zVF}{RT})\right]}{1-\exp(-\frac{zVF}{RT})}. \tag{3}$$

[1] PhD student, Applied Sciences and Computer Engineering, Mechanics, specialization Applied Mechanics, e-mail: vacibera@ntc.zcu.cz

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Results, Conclusion

Resistance coefficient and diffusion coefficient can be easy expressed from equation (1), respectively (3). Both of these coefficient were computed in the range of $-50 \; - \; 50 \; mV$ *for one sodium channel*. As seen on the Fig.1 and Fig.2 resistance coefficient from equation (1) has values in the order of 10^{20}. Diffusion coefficient has values in the order of 10^{-24} for one sodium channel.

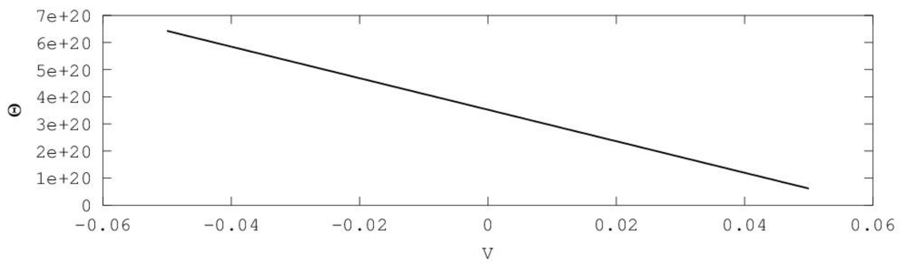

Figure 1: Approximate values of resistance coefficient Θ in equation (1)

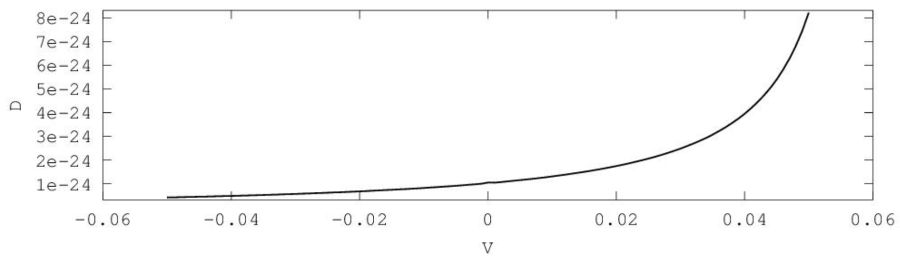

Figure 2: Approximate values of diffusion coefficient D in Nernst - Planck equation (2)

It is worth to notice, that these results are only rough and can vary in the dependence on type of channel and kind of ion. Both of the considered equations use continuous approach. Unfortunately, it is very probable, that continuous approach is not fulfilled for ion channels description. Future research should therefore concentrate on the investigation of discontinuous description also. It would be interesting to investigate use of Langevin equation, because it allows to include also Brownian motion of the channel walls and other features into the mathematical model.

Acknowledgement

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