Numerical Model of Ions Transport in Biomembrane Channel

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Abstract **The paper deals with the numerical model of the ions permeation in potassium channels of biomembrane. For stationary Schrodinger-Poisson model derived in [3] we formulate two variational Galerkin's identities for electric scalar potential φ and wave function u. By using finite element approximation we obtain iteration system of algebraic equations.**

Keywords **Ion Transport, Finite Element Approximation, Poisson-Schrödinger model.**

I. Poisson-Schrödinger Model - Ion Channel Transport

For the stationary Poisson-Schrödinger model [1, 2, 4] electric potential φ and wave function u fulfill system of equations

$$-\frac{\hbar}{2m}\nabla^2 u + q\varphi u = 0 \tag{1}$$

$$\nabla \circ (\varepsilon \nabla \otimes \varphi) = -qu^2 \tag{2}$$

For presented ion channel

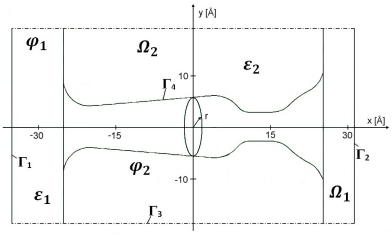

Fig. 1. Scheme of the ion channel

the mixed boundary conditions of Dirichlet-Neumann type are

$$\varphi = 0|_{\Gamma_1}; \quad \varphi = U = 120[mV]|_{\Gamma_2}; \quad \frac{\partial \varphi}{\partial n} = 0|_{\Gamma_3} \tag{3}$$

$$\varphi_1 = \varphi_2; \quad \varepsilon_1 \frac{\partial \varphi_1}{\partial n} - \varepsilon_2 \frac{\partial \varphi_2}{\partial n} = 0|_{\Gamma_4} \tag{4}$$

The problem (1)-(2) with boundary conditions (3)-(4), we will transform to two Galerkin's variational identities

$$\int_\Omega (\nabla \otimes u) \circ (\nabla \otimes v) dV + \int_\Omega qu\varphi v dV = \\ = \int_\Omega vg(u) dV + \oint_{\partial\Omega} (v\nabla \otimes u) \circ dS \tag{5}$$

$$\int_\Omega (\varepsilon\nabla \otimes \varphi) \circ (\nabla \otimes v) dV = \\ = \int_\Omega qu^2 dV + \oint_{\partial\Omega} (v(\varepsilon\nabla \otimes \varphi) \circ dS \tag{6}$$

where u, φ are trial functions and v is test function. Applied to (5) and (6) the finite element approximation

$$\varphi^e(x,y) = \sum N^e_\alpha(x,y)\varphi^e_\alpha \tag{7}$$

where e is number of elements, $\alpha = i, j, k$ is node number, this system will take the form

$$[K_1]\{u\}^{k+1} + [K_2]\{u,\varphi\}^{k+1} = [F_1]^{k+1}\{u\}^{k+1} = 0 \tag{8}$$

$$[K_3]\{\varphi\}^k = [F_2]\{u\}^k \tag{9}$$

Using Python, GMSH and FEniCS programs [5] we get the following result for the zero-iteration of scalar potential distribution φ

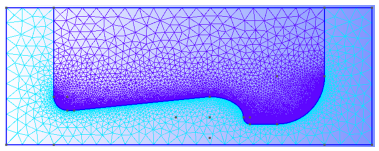

Fig. 2. Mesh example generated in GMSH2.6

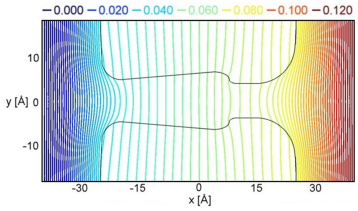

Fig. 3. Distribution of potential field for $\varepsilon_1 < \varepsilon_2$

II. Conclusion

This way of solving the system of equations by iterative method allows to determine the potential distribution, the density of energy and ion flux, which is an electric current flowing through the channel.

References

[1] Hille, H.: "Ionic Channels of Exitable Membranes", Sinaure Assoc. Inc., Sunderland, Mass. 1992.
[2] Roux, B., Allen, T., Bemeche, S., Im, W.: "Theoretical and Computational Models of Biological Ion Chennels", Quarterly Reviews of Biophysics 37, 1 (2004), pp. 15-103, Cambridge University Press.
[3] Krzemiński S. K., Przybylski P.: "Quantum Dynamics for Ion Channel Transport, Poisson-Schrödinger Modell". Przegląd Elektrotechniczny NR 6, pp. 263-265. Warszawa 2013.
[4] Vaziri, A., Plenio, M.B.: "Quantum coherence in ion channels". New Journal of Physics, Vol. 12, pp. 1-17, 2010.
[5] Logg, A., Mardal, K.-E., Wells, G.:"Automated Solution of Differential Equations by the Finite Element Method", 2012.