VILNIAUS UNIVERSITETAS
MATEMATIKOS IR INFORMATIKOS FAKULTETAS
PROGRAMŲ SISTEMŲ KATEDRA

Selektyvios membranos modeliavimas amperometriniame biojutiklyje

*angl. pav.

Kursinis darbas

Atliko:	4 kurso 1 grupės studentas Kęstutis Gimbutas	(parašas)
Darbo vadovas:	prof. habil. dr. Romas Baronas	(parašas)

Vilnius – 2014

Turinys

Įvadas

<Tektas> *.

1. Mono-Layer Mono-Enzyme Model of Biosensor

Formules were taken from [BIKK09].

1.1. Mathematical Model

According to simplified scheme, the substrate (S) binds to the enzyme (E) and is converted to poduct (P),

$$S \xrightarrow{E} P \tag{1}$$

$$\begin{aligned} \frac{\delta S}{\delta t} &= D_S \frac{\delta^2 S}{\delta x^2} - \frac{V_{max} S}{K_M + S}, \\ \frac{\delta P}{\delta t} &= D_P \frac{\delta^2 P}{\delta x^2} + \frac{V_{max} S}{K_M + S}, \ x \in (0; d), \ t > 0 \end{aligned} \tag{2}$$

1.2. Initial and Boundary Conditions

$$\begin{aligned} &S(x,0) = 0, x \in [0; d), \\ &S(d,0) = S_0, \end{aligned} \tag{3}$$

$$\begin{aligned} &P(x,0) = 0, x \in [0; d), \\ &P(d,0) = P_0, \end{aligned} \tag{4}$$

$$P(0;t) = 0, \ t > 0. \tag{5}$$

$$D_S \frac{\delta S}{\delta x}\bigg|_{x=0} = 0, t > 0. \tag{6}$$

$$\frac{\delta S}{\delta x}\bigg|_{x=0} = 0, t > 0. \tag{7}$$

$$S(d,t) = S_0, t > 0, \tag{8}$$

$$P(d,t) = P_0, t > 0. \tag{9}$$

1.3. Characteeristics of the Biosensor Response

1.3.1. Response Time

$$T = \min_{i(t)>0} \left\{ t : \frac{t}{i(t)} \left| \frac{d_i(t)}{dt} \right| < \epsilon \right\} \tag{10}$$

1.4. Numerical Approximation of Equations

1.4.1. Implicit Scheme

$$\begin{aligned}
&\frac{S_i^{j+1} - S_i^j}{\tau} = D\frac{S_{i+1}^{j+1} - 2S_i^{j+1} + S_{i-1}^{j+1}}{h^2} - \frac{V_{max}S_i^j}{K_M + S_i^j},\\
&\frac{P_i^{j+1} - P_i^j}{\tau} = D\frac{P_{i+1}^{j+1} - 2P_i^{j+1} + P_{i-1}^{j+1}}{h^2} + \frac{V_{max}S_i^j}{K_M + S_i^j},\\
&i = 1, ..., N-1, j = 0, ..., M-1.
\end{aligned} \tag{11}$$

1.4.2. Initial and Boundry Condtitions

$$\begin{aligned}
&S_i^0 = 0, i = 0, ..., N-1,\\
&S_N^0 = S_0,
\end{aligned} \tag{12}$$

$$\begin{aligned}
&P_i^0 = 0, i = 0. ..., N-1,\\
&P_N^0 = P_0
\end{aligned} \tag{13}$$

$$S_0^j = S_1^j, S_N^j = S_0, j = 1, ..., M, \tag{14}$$

$$P_0^j = 0, P_N^j = P_0, j = 1, ..., M, \tag{15}$$

1.4.3. Calculation Procedure

$$i(t_j) \approx t_j = n_e F D_p P_i^j / h, \, j = 1, ..., M. \tag{16}$$

1.5. Validation of Numerical Solution

1.5.1. Inicial Conditions of Calculations

$$
\begin{aligned}
&S_0 = 1\mu M,\, P_0 = 0\mu M,\\
&D_s = 300\mu m^2/s,\, D_p = 300\mu m^s/s,\\
&T = 50s,\;\; d_1 = 10\mu m,\, d_2 = 15\mu m,\, d_3 = 100\mu m; d_4 = 150\mu m,\\
&\tau = 0.1s,\, h = 0.1\mu m,\\
&V_{max} = 100\mu M/s,\, \epsilon = 0.05,\\
&F = 961485,\, K_M = 100\mu M,\, n_e = 2.
\end{aligned}
\tag{17}
$$

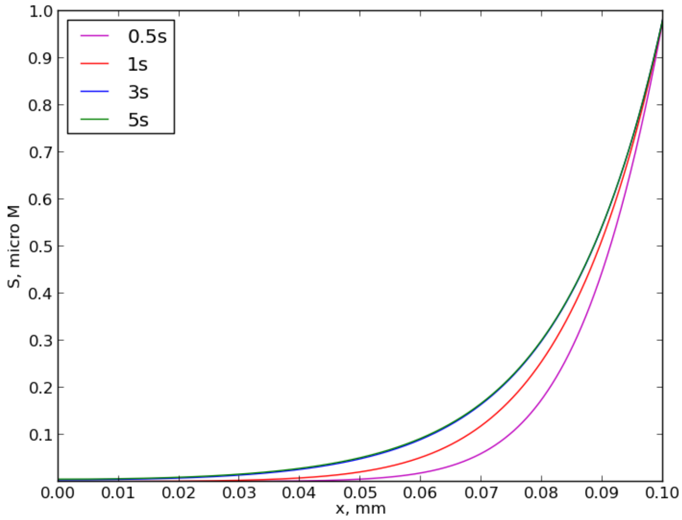
1.5.2. Obtained Matrixes from the Given Implicit Scheme

Used: Finite Difference Solution, Implicit Scheme. Solved using Tridiagonal Matrix Algorythm.

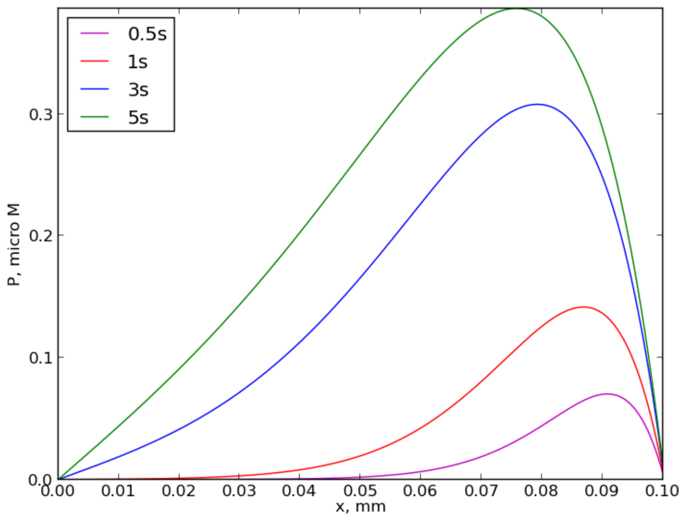
$$
\begin{cases}
S_{i+1}^{j+1} - S_i^{j+1}\left(1 + \dfrac{h^2}{D\tau}\right) = \dfrac{h^2}{D\tau}\left(\dfrac{V_m ax S_i^j \tau}{K_M + S_i^j} - S_i^j\right), \, when\ j = 0,\\
\cdots\ ,\\
S_{i-1}^{j+1} - S_i^{j+1}\left(2 + \dfrac{h^2}{D\tau}\right) + S_{i+1}^{j+1} = \dfrac{h^2}{D\tau}\left(\dfrac{V_m ax S_i^j \tau}{K_M + S_i^j} - S_i^j\right), \, when\ j = 1, ..., M-1,\\
\cdots\ ,\\
S_0 + S_{i-1}^{j+1} - S_i^{j+1}\left(2 + \dfrac{h^2}{D\tau}\right) = \dfrac{h^2}{D\tau}\left(\dfrac{V_m ax S_i^j \tau}{K_M + S_i^j} - S_i^j\right), \, when\ j = M.
\end{cases}
\tag{18}
$$

$$
\begin{cases}
P_{i+1}^{j+1} - P_i^{j+1}\left(2 + \dfrac{h^2}{D\tau}\right) = \dfrac{h^2}{D\tau}\left(-P_i^j - \dfrac{V_m ax S_i^j \tau}{K_M + S_i^j}\right), \, when\ j = 0,\\
\cdots\ ,\\
P_{i-1}^{j+1} - P_i^{j+1}\left(2 + \dfrac{h^2}{D\tau}\right) + P_{i+1}^{j+1} = \dfrac{h^2}{D\tau}\left(\dfrac{V_m ax S_i^j \tau}{K_M + S_i^j} - S_i^j\right), \, when\ j = 1, ..., M-1,\\
\cdots\ ,\\
P_0 + P_{i-1}^{j+1} - P_i^{j+1}\left(2 + \dfrac{h^2}{D\tau}\right) = \dfrac{h^2}{D\tau}\left(\dfrac{V_m ax S_i^j \tau}{K_M + S_i^j} - S_i^j\right), \, when\ j = M.
\end{cases}
\tag{19}
$$

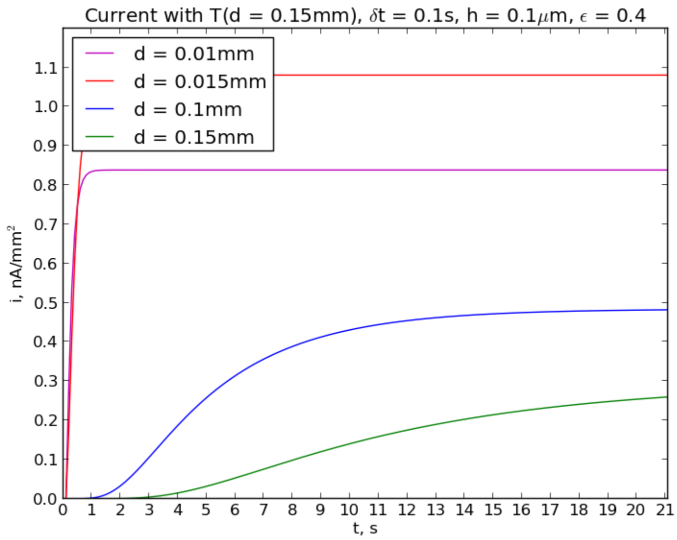
1.5.3. Results



1 pav.: Substrate



2 pav.: Product



3 pav.: Current

Literatūros sąrašas

[BIKK09] Romas Baronas, Feliksas Ivanauskas, IU IU Kulis, and Juozas Kulys. *Mathematical modeling of biosensors: an introduction for chemists and mathematicians*, volume 9. Springer, 2009.