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COMPUTER MODELLING OF BIOSENSOR WITH PRODUCT INHIBITION

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ABSTRACT

The computer model of a one-dimensional-in-space amperometric biosensor is studied in this paper [6, 7]. The model is based on diffusion equations containing a non-linear term related to Michaelis-Menten kinetics of the enzymatic reactions in the case of the product inhibition [3]. The model takes into account the mass transport in the diffusion layer and the reaction kinetics with the mass transport in the enzyme layer. We consider a reaction scheme in wich the enzyme (E) interacts with the substrate (S) to form reversible enzyme-substrate complex (ES). The complex ES splits into the free enzyme and the product (P). The enzyme is inhibited by the product to form the enzyme-product complex (EP),

$$\mathrm{E} + \mathrm{S} \longleftrightarrow \mathrm{ES} \longrightarrow \mathrm{E} + \mathrm{P}, \tag{1}$$

$$\mathrm{E} + \mathrm{P} \longleftrightarrow \mathrm{EP}. \tag{2}$$

Assuming the quasi-steady-state approximation, the process in the enzyme layer is described by a following reaction-diffusion equations:

$$\frac{\partial S_e}{\partial t} = D_{Se}\frac{\partial^2 S_e}{\partial x^2} - \frac{V_{max} S_e}{K_M + S_e + \frac{K_M P_e}{K_P}}, \tag{3}$$

$$\frac{\partial P_e}{\partial t} = D_{Pe}\frac{\partial^2 P_e}{\partial x^2} + \frac{V_{max} S_e}{K_M + S_e + \frac{K_M P_e}{K_P}}, \tag{4}$$

where S_e and P_e stand for the concentrations of the substrate and product respectively in the enzyme layer, D_{Se}, D_{Pe} are the diffusion coeficients, V_{max} is the maximal enzymatic rate, K_M is the Michaelis-Menten constant, K_P is the inhibition constant, x and t stand for space and time [1, 4]. The mass transport in the diffusion layer, initial and boundary conditions as well as the equation of the biosensor response are defined similarly in the paper [4].

Stated problem was solved numerically using finite difference method [2, 5].

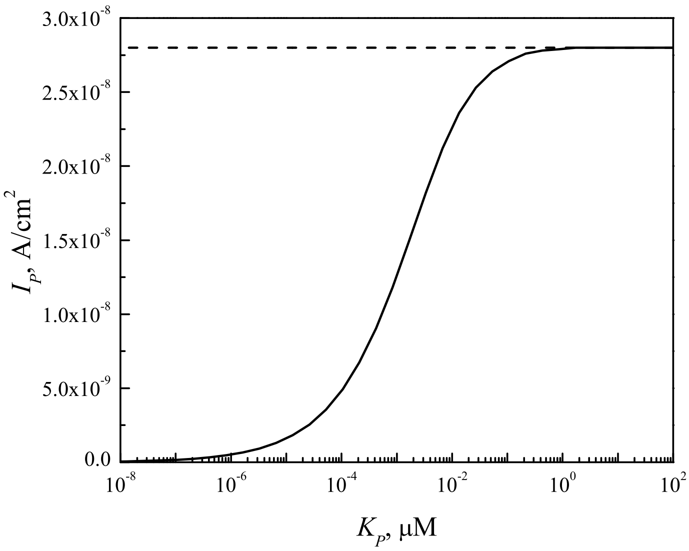

Figure 1: The dependence of the density I_P of the steady state current on the inhibition coeficient K_P (solid line). The current density calculated without the enzyme inhibition by the product is represented by the dashed line.

The effect of the product inhibition on the response of the biosensor is presented in Fig. 1. The limiting current density representing the case when no product inhibition is observed is shown by the dashed line. The current density grows as the inhibition constant increases and reaches the limiting current density.

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