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COMPUTATIONAL MODELLING OF BIOSENSOR-BASED ANALYTICAL SYSTEMS

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Biosensors are sensing devices made up of a combination of a specific biological entity, usually an enzyme, that recognizes a specific target analyte and a transducer that translates the bio-recognition event into an electrical signal [1]. The signal is usually proportional to the concentration of the analyte (substrate). The biosensors are reliable, cheap and sensitive for environmental, clinical and industrial applications. Practical biosensors form sandwich-like structures. An electrode acting as a transducer is covered by a selective membrane following a layer of the immobilized enzyme and an outer porous or perforated membrane.

To improve the efficiency of the design of an analytical system and to optimize its configuration, a model of a certain biosensor should be build. In the enzyme region, the enzyme-catalysed reaction is coupled with the mass transport by diffusion and is described by a system of non-linear reactiondiffusion equations [2; 3]. Assuming the quasi steady state approximation the dynamics of the biosensor action can be described as follows:

$$\frac{\partial S}{\partial t} = D_S \Delta S - \frac{V_{max}S}{K_M + S}, \quad \frac{\partial P}{\partial t} = D_P \Delta P + \frac{V_{max}S}{K_M + S},\tag{1}$$

where Δ is the Laplacian, S is the substrate concentration, P is the concentration of the reaction product, V_{max} is the maximal enzymatic rate, K_M is the Michaelis constant. Outside the enzyme region only the mass transport by diffusion is considered. The porous membrane was assumed as a periodic media, and a homogenization process was applied. The governing equations together with appropriate initial, boundary and matching conditions form a boundary-value problem, which was solved numerically by applying the finite difference technique.

The biosensor geometry and the catalytic parameters significantly influence the sensitivity and stability of the biosensors [1]. The numerical simulation was applied to investigate pecularities of the biosensors response and to optimize the biosensors characteristics [2; 3].

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