

# COMPUTATIONAL MODELLING OF AMPEROMETRIC BIOSENSORS IN THE CASE OF SUBSTRATE AND PRODUCT INHIBITION

DAINIUS ŠIMELEVIČIUS

*Department of Software Engineering, Vilnius University*

Naugarduko 24, 03225 Vilnius, Lithuania

E-mail: dainius.simelevicius@mif.vu.lt

An amperometric biosensor is a device used for measuring concentration of some specific chemical or biochemical substance in a solution [1]. Biosensors use specific biochemical reactions catalyzed by enzymes immobilized on electrodes. Once a product of a reaction reaches an electrode it oxidizes or reduces producing the anodic current which is measured.

The response of an amperometric biosensor at mixed enzyme kinetics and diffusion limitations has been modelled digitally in the case of substrate and product inhibition. The model is based on non-stationary diffusion equations containing a non-linear term related to non-Michaelis-Menten kinetics of the enzyme reaction [2].

The simulation of the biosensor response has been carried out using the finite difference technique [3]. The mathematical model and the numerical solution were validated using analytical solutions existing for the very specific cases of the model parameters [1; 2].

The dimensionless model of the biosensor with substrate and product inhibition has been constructed in order to decrease the number of biosensor properties. Governing equations in biosensor's enzyme layer in dimensionless coordinates are expressed as follows:

$$\frac{\partial S}{\partial T} = \frac{\partial^2 S}{\partial X^2} - \Phi^2 \frac{S}{(1 + P/K_p) + S(1 + S/K_s)}, \quad (1)$$

$$\frac{\partial P}{\partial T} = \frac{D_{p_e}}{D_{s_e}} \frac{\partial^2 P}{\partial X^2} + \Phi^2 \frac{S}{(1 + P/K_p) + S(1 + S/K_s)}, \quad (2)$$

where  $T$  stands for the time,  $X$  is the space,  $S$  is the substrate concentration,  $P$  is the product concentration,  $D_{s_e}$  and  $D_{p_e}$  are diffusion coefficients,  $K_p$  and  $K_s$  are product and substrate inhibition rates, respectively,  $\Phi^2$  is the diffusion modulus.

The dimensionless model has been used to investigate the biosensor behaviour in a set of numerical experiments. The sensitivity of biosensor at different values of substrate and product inhibition rate at different substrate concentrations has been analyzed.

## REFERENCES

- [1] H. Gutfreund. *Kinetics for the Life Sciences*. Cambridge University Press, Cambridge, 1995.
- [2] J. Kulys and R. Baronas. Modelling of Amperometric Biosensors in the case of substrate inhibition. *Sensors*, **6** 2006, 1513 – 1522.
- [3] A.A. Samarskii. *The Theory of Difference Schemes*. Marcel Dekker, New York-Basel, 2001.