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Computational Analysis of Mechanisms Governing the Sensitivity and Efficiency of Enzyme-Based Biosensors and Bioreactors

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Enzymes play a crucial role in analytical biosensing systems due to their ability to specifically recognize analytes (substrates) and catalyse their conversion into products that can be readily detected using conventional analytical methods, such as electrochemical, optical, and other techniques [1]. In such systems, enzymes are primarily used in immobilized forms as biosensors or bioreactors. Enzyme-based biosensors and bioreactors are widely used in various fields, including medical and clinical diagnostics, environmental monitoring, as well as industrial and biotechnological processes [2, 3]. Computational modelling of enzyme-based biosensors and bioreactors enables the simulation of biosensor responses and bioreactor yields under both steady-state and transient conditions. The simulations consider biosensors and bioreactors with complex geometries and kinetic schemes that describe the action of biocatalysts. Mathematical and computational tools are widely used to optimize existing biochemical systems and to develop novel ones [4]. The aim of this work was to investigate the influence of the partitioning and diffusion limitations on the efficiency of enzyme-based bioreactors and biosensors using a three-layer model involving different schemes of the enzyme kinetics [5-7]. Exact steady state analytical solutions for the substrate and reaction product concentrations and the bioreactor effectiveness, as well as biosensor response, were obtained for the first and zero-order reaction rates. The transient action of enzyme-based bioreactors and amperometric as well as potentiometric biosensors was numerically investigated using the finite difference technique. The numerical simulator has been programmed in Java. Mathematical modelling of the diffusion-limited membrane and the conditions under which

the same values of the steady state characteristics are obtained when simulating the treated system by purposefully changing the values of the diffusion and distribution coefficients have been investigated [5, 6]. The application of different specific types of interface conditions, perfect contact and partition conditions, at which the steady state biosensor response is the same for both types of interface conditions, has been studied. To simplify the analysis, effective diffusion coefficients for the overall layer, comprising the diffusion-limiting membrane and the outer diffusion (Nernst) layer, have been identified to reduce the three-layer model to an equivalent two-layer model [5, 6]. In particular, it was determined that at relatively high substrate concentrations and in the presence of external diffusion limitation, the transient response of an amperometric biosensor exhibiting uncompetitive substrate inhibition may follow a five-phase pattern, depending on the model parameter values. Specifically, the response starts from zero, reaches a global or local maximum, decreases to a local minimum, increases again, and finally decreases to a steady intermediate value [7]. Managing such oscillations in the transient biosensor response is crucial for accurately predicting the analyte concentration, e.g., glucose in human blood, using a glucose biosensor.

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