Mechanistic modeling of cyclic voltammetry: A helpful tool for understanding biosensor principles and supporting design optimization

Abstract Design, optimization and integration of biosensors hold a great potential for the development of cost-effective screening and point-of-care technologies. However, significant progress in this field can still be obtained on condition that sufficiently accurate mathematical models will be developed. Herein, we present a novel approach for the improvement of mechanistic models which do not only combine the fundamental principles but readily incorporate the results of electrochemical and morphological studies. The first generation glucose biosensors were chosen as a case study for model development and to perform cyclic voltammetry (CV) measurements. As initial step in the model development we proposed the interpretation of experimental voltammograms obtained in the absence of substrate (glucose). The model equations describe dynamic diffusion and reaction of the involved species (oxygen, oxidized/reduced forms of the mediator - Prussian Blue/Prussian White). Furthermore, the developed model was applied under various operating conditions as a crucial tool for biosensor design optimization. The obtained qualitative and quantitative dependencies towards amperometric biosensors design optimization were independently supported by results of cyclic voltammetry and multi-analytical studies, such as scanning electron microscopy (SEM), energy dispersive X-ray spectroscopy (EDX) and liquid chromatography-electrospray ionization-tandem mass spectrometry (LC-ESI-MS/MS). Remarkably, a linear response of the optimized biosensors tested at the applied voltage (~0.14V) in the presence of the glucose was obtained from 10^{-3} to 10^{-5}M (relative standard deviation (RSD) <7% per electrode). We believe that the presented model can be used to determine the exact mechanism driving the electrochemical reactions and to identify critical system parameters affecting the biosensor response that would significantly contribute to the knowledge on biosensing, devices design and bioengineering strategies in the future.

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