Simulation Protocol of Simple Diffusional Electrode Mechanism in Square-Wave Voltammetry

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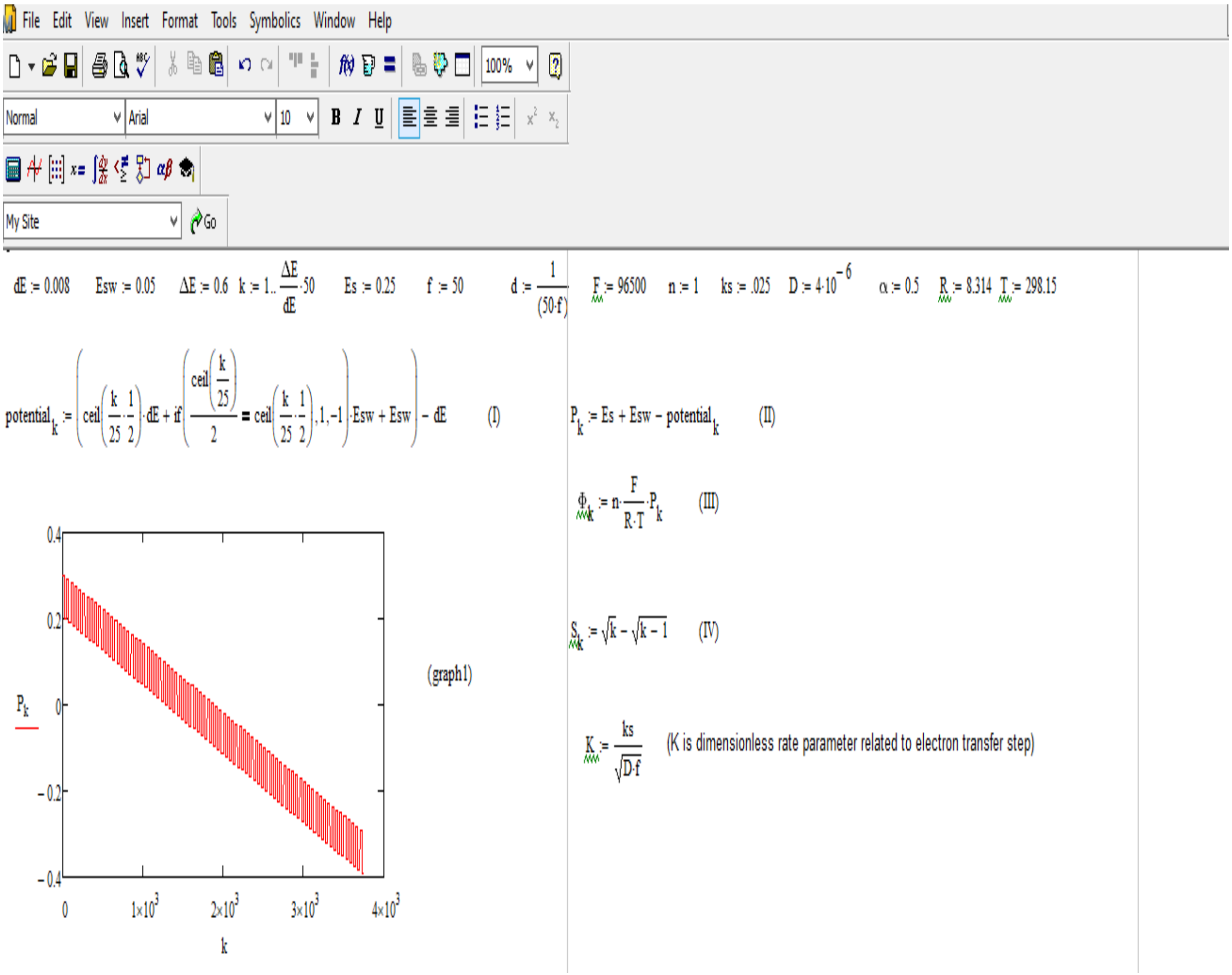
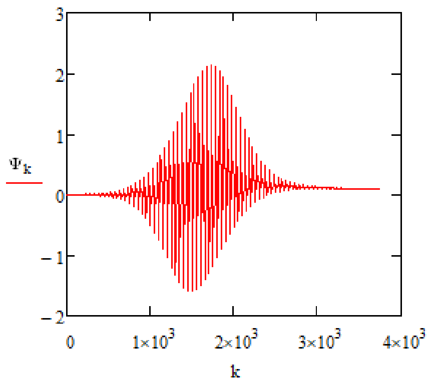
Abstract

A working protocol for calculation of square-wave voltammograms of a simple diffusional electrode transformation of water soluble redox couple is presented in the simulation package MATHCAD. We give the readers all parameters and the recursive formula needed to calculate the voltammograms of this electrode mechanism relevant to describe the voltammetric behavior of many water-soluble proteins and enzymes.



$$\Psi_1 := \frac{K \cdot e^{-\alpha \cdot \Phi_1}}{1 + 2 \cdot K \cdot \left[(50 \cdot \pi)^{-\frac{1}{2}} \cdot \left(1 + e^{\Phi_1}\right) \right] \cdot e^{-\alpha \cdot \Phi_1}} \qquad \text{(V)} \qquad \Psi_k := \frac{K \cdot e^{-\alpha \cdot \Phi_k} \cdot \left[1 - 2 \cdot (50 \cdot \pi)^{-\frac{1}{2}} \cdot \left(1 + e^{\Phi_k}\right) \cdot \sum_{j=1}^{k-1} \left(\Psi_j \cdot S_{k-j+1} \right) \right]}{1 + 2 \cdot K \cdot \left[(50 \cdot \pi)^{-\frac{1}{2}} \cdot \left(1 + e^{\Phi_k}\right) \right] \cdot e^{-\alpha \cdot \Phi_k}}$$

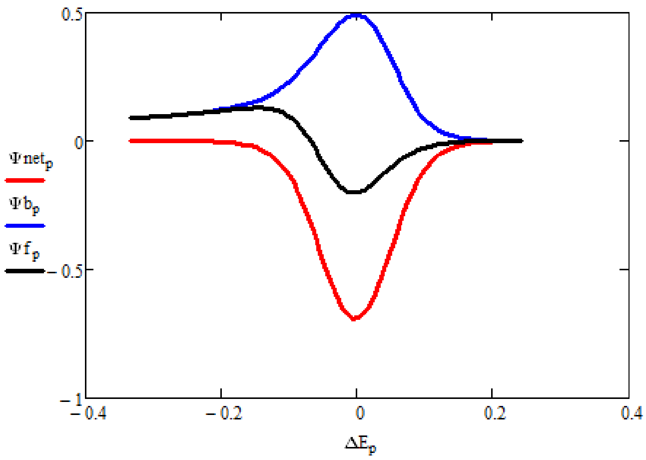


(graph2)

$$p := 1 .. \frac{\Delta E}{dE} - 2$$

$$\Psi b_p := \Psi_{(p+1) \cdot 50} \quad \text{(VII)} \qquad \Psi f_p := \Psi_{50 \cdot p + 25} \quad \text{(VIII)} \qquad \Psi net_p := \Psi f_p - \Psi b_p \quad \text{(IX)}$$

$$\Delta E_p := Es - (p) \cdot dE \quad \text{(X)}$$



(graph3)

$\underset{\sim}{A} := 0.0314 \qquad cOx := 1\cdot10^{-6}$

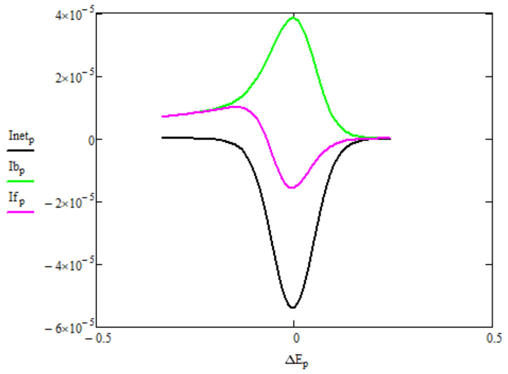
(XI) (XII)

$$If_p := \frac{(\Psi f)_p}{0.55}\cdot F\cdot A\cdot\sqrt[2]{D\cdot f}\cdot cOx \qquad \text{(XIII)}$$

$$Ib_p := \frac{(\Psi b)_p}{0.55}\cdot F\cdot A\cdot\sqrt[2]{D\cdot f}\cdot cOx \qquad \text{(XIV)}$$

$$Inet_p := If_p - Ib_p \qquad \text{(XV)}$$

$\Psi net_p =$	$\Psi f_p =$	$\Psi b_p =$	$\Delta E_p =$
$-5.065\cdot10^{-4}$	$-9.165\cdot10^{-5}$	$4.148\cdot10^{-4}$	0.242
$-6.997\cdot10^{-4}$	$-1.511\cdot10^{-4}$	$5.487\cdot10^{-4}$	0.234
$-9.579\cdot10^{-4}$	$-2.189\cdot10^{-4}$	$7.39\cdot10^{-4}$	0.226
$-1.309\cdot10^{-3}$	$-3.063\cdot10^{-4}$	$1.002\cdot10^{-3}$	0.218
$-1.786\cdot10^{-3}$	$-4.225\cdot10^{-4}$	$1.363\cdot10^{-3}$	0.21
$-2.436\cdot10^{-3}$	$-5.788\cdot10^{-4}$	$1.857\cdot10^{-3}$	0.202
$-3.321\cdot10^{-3}$	$-7.899\cdot10^{-4}$	$2.531\cdot10^{-3}$	0.194
$-4.526\cdot10^{-3}$	$-1.075\cdot10^{-3}$	$3.451\cdot10^{-3}$	0.186
$-6.162\cdot10^{-3}$	$-1.46\cdot10^{-3}$	$4.702\cdot10^{-3}$	0.178
$-8.383\cdot10^{-3}$	$-1.979\cdot10^{-3}$	$6.405\cdot10^{-3}$	0.17
-0.011	$-2.677\cdot10^{-3}$	$8.714\cdot10^{-3}$	0.162
-0.015	$-3.613\cdot10^{-3}$	0.012	0.154
-0.021	$-4.864\cdot10^{-3}$	0.016	0.146
-0.028	$-6.529\cdot10^{-3}$	0.022	0.138
-0.038	$-8.731\cdot10^{-3}$	0.029	0.13
...	...	...	...



(graph4)

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