MATHCAD FILE FOR SIMULATION OF SIMPLE DIFFUSIONAL

Ox + ne = Red MECHANISM IN

SQUARE WAVE VOLTAMMETRY

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Abstract

We provide the readers entire >MATHCAD working sheet for simulation of square wave voltammograms of simple Ox + ne- = Red reaction under conditions of square-wave voltammetry. Model is suitable to study the features of quasireversible electrode systems in which belong many metal ions, hydrophilic drugs and water-soluble proteins.

DIFFUSIONAL SIMPLE ELECTRODE REACTION

MATHCAD – QUASIREVERSIBLE in SQUARE WAVE VOL

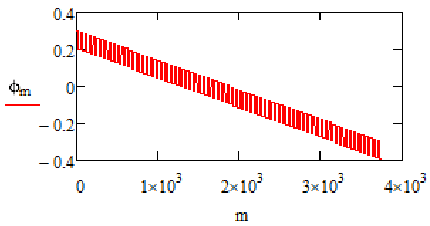
OX + ne = Red
dissolved states
K is dimensionless kinetic parameter
ks is standard rate constant of electron transfer
f is SW frequency
α is electron transfer coefficient
Φ is dimensionless potential
Esw is square wave amplitude
dE is potential increment
Ψ is dimensionless current
S is numerical integration factor

$dE := 0.008 \quad Esw := 0.05 \quad \Delta E := 0.6 \quad m := 1 .. \frac{\Delta E}{dE} \cdot 50 \quad Es := 0.25 \quad i := 1 .. 1$

$f := 50$

$$relativenpot_m := \left(\mathrm{ceil}\left(\frac{m}{25}\cdot\frac{1}{2}\right)\cdot dE + \mathrm{if}\left(\frac{\mathrm{ceil}\left(\frac{m}{25}\right)}{2} = \mathrm{ceil}\left(\frac{m}{25}\cdot\frac{1}{2}\right), 1, -1\right)\cdot Esw + Esw\right) \quad \phi_m := Es + Esw - relativenpot_m$$

$ks := .008 \quad D := 4\cdot 10^{-6}$



$$K := \frac{ks}{\sqrt{D\cdot f}} \qquad \alpha := 0.5$$

$K_i =$

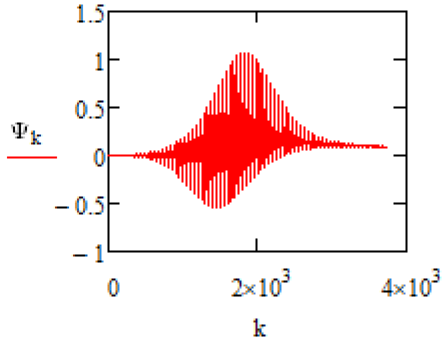
$\log(K_i) =$

$F := 96500 \quad n := 1 \quad R := 8.314 \quad T := 298.15 \quad \Phi_m := n\cdot\frac{F}{R\cdot T}\cdot\phi_m$

$$\Psi_1 := \frac{K\cdot e^{-\alpha\cdot\Phi_1}}{1 + 2\cdot K\cdot\left[(50\cdot\pi)^{-\frac{1}{2}}\cdot\left(1 + e^{\Phi_1}\right)\right]\cdot e^{-\alpha\cdot\Phi_1}}$$

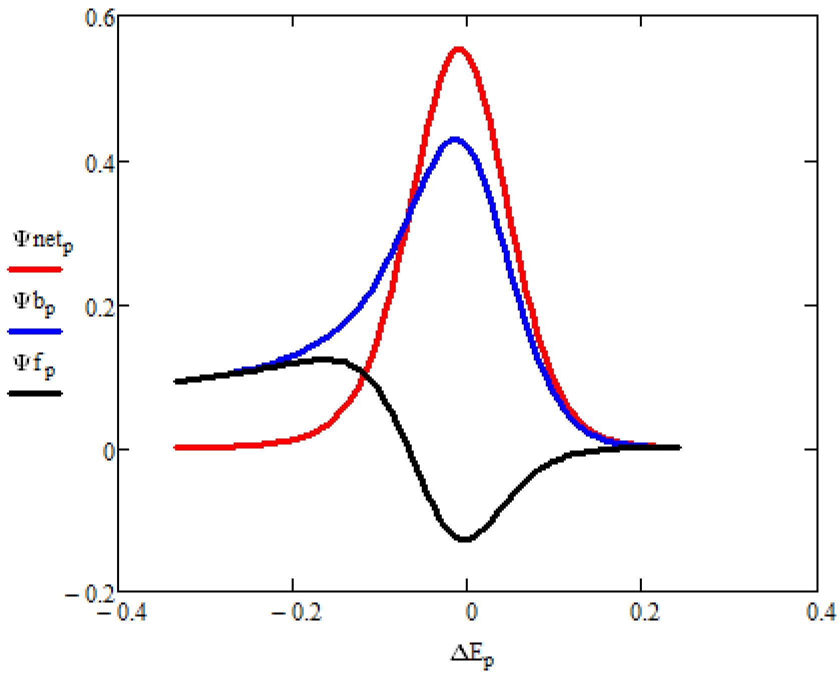
$k := 1 .. \frac{\Delta E}{dE}\cdot 50 \quad S_k := \sqrt{k} - \sqrt{k-1}$

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



$$p := 1 .. \frac{\Delta E}{dE} - 2 \quad \Psi b_p := \Psi_{(p+1)\cdot 50} \quad \Psi f_p := \Psi_{50\cdot p+25} \quad \Psi net_p := \Psi b_p - \Psi f_p$$

$$\Delta E_p := Es - (p)\cdot dE$$



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