Inhibition of the Initial Form of Water-Soluble Redox Enzymes-Theoretical Consideration under Conditions of Square-Wave Voltammetry (MATHCAD File)

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$Es := 0.4 \quad \Delta E := 0.8 \quad dE := 0.004 \quad Esw := 0.05$

$n := 1 \quad F := 96500 \quad R := 8.314 \quad T := 298.15$

$D := 0.000005$

$kc := 30055.2500$

$f := 10$

$ks := 10^{-.150504499512}$

Model of Diffusional Electrode Mechanism with Irreversible Chemical Reaction Coupled to Initial Redox Form in Square-Wave Voltammetry

$j := 1 .. \frac{\Delta E}{dE} \cdot 50$

$\alpha := 0.5$

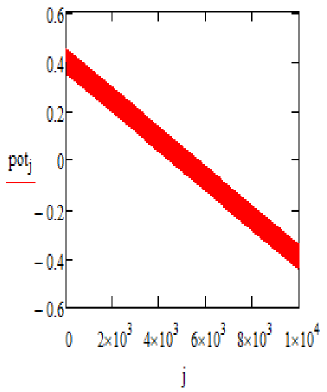
$pot_j := Es + Esw - \left[\left(ceil\left(\frac{j}{25} \cdot \frac{1}{2}\right) \cdot dE + if\left(\frac{ceil\left(\frac{j}{25}\right)}{2} = ceil\left(\frac{j}{25} \cdot \frac{1}{2}\right), 1, -1\right) \cdot Esw + Esw\right) - dE\right]$

$Ket := \frac{ks}{f^{0.5} \cdot D^{0.5}}$

$Ket = 100.002$

$Kchem := \frac{kc}{f}$

$Kchem = 3.006 \times 10^3$



$k := 1 .. \frac{\Delta E}{dE} \cdot 50$

$S_k := \sqrt{k} - \sqrt{k-1}$

$\Phi_j := n \cdot \frac{F}{R \cdot T} \cdot pot_j$

$L_k := erfc\left[\left(Kchem \cdot \frac{k}{50}\right)^{0.5}\right] - erfc\left[\left[Kchem \cdot \frac{(k-1)}{50}\right]^{0.5}\right]$

Definitions and Meanings of the Symbols

f is the SW frequency
ks is standard rate constant of electron transfer
α is electron transfer coefficient
n is number of exchanged electrons
dE is potential step
Esw is square-wave amplitude
T is thermidynamic teperature
R is universal gas constant
kc is rate constant of irreversible chemical rection
Ket is dimensionless kinetic electrode parameter
Kchem is dimensionless kinetic chemical parameter
Sk is numerical integration factor
Es is starting potential
Φ is dimensionless potentials
F is the Faraday constant
Ψ is dimensionless current

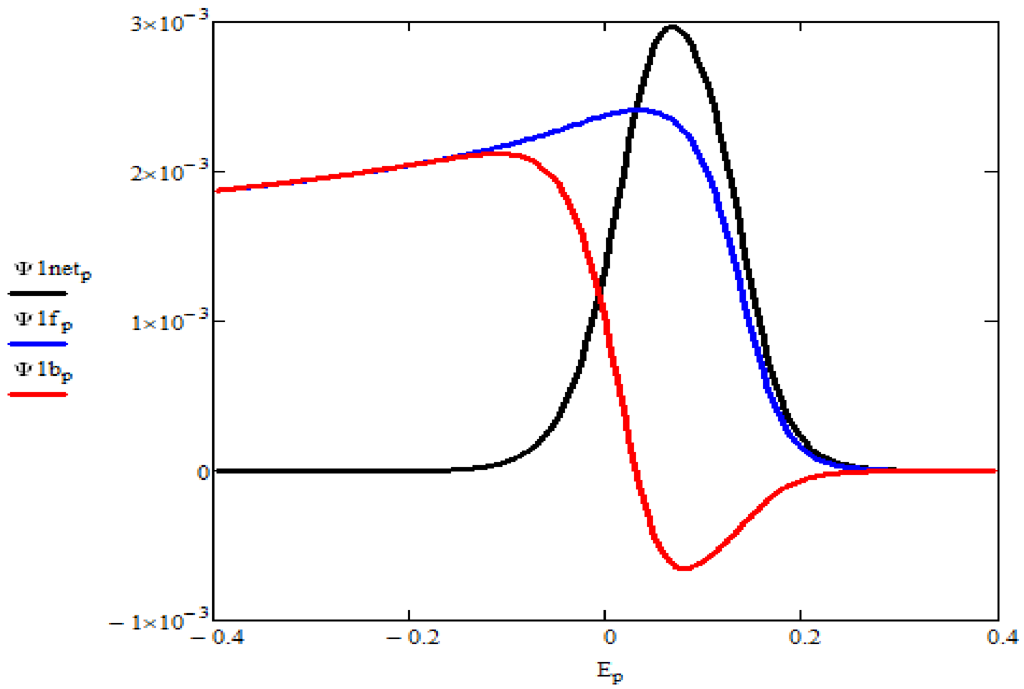
$$\Psi 1_1 := \frac{\dfrac{Ket \cdot e^{-\alpha \cdot \Phi_1}}{(50 \cdot \pi)^{0.5}} - \left[2Ket \cdot e^{-\alpha \cdot \Phi_1} \cdot \dfrac{\left(1 + e^{\Phi_1}\right)}{(50 \cdot \pi)^{0.5}} \cdot 0 + \dfrac{Kchem^1 \cdot e^{-\alpha \cdot \Phi_1} \cdot 1 \cdot L_1}{(50 \cdot \pi)^{0.5}} \right]}{1 + \dfrac{2Ket \cdot e^{-\alpha \cdot \Phi_1} \cdot \left(1 + e^{\Phi_1}\right) \cdot S_1}{(50 \cdot \pi)^{0.5}} - \dfrac{Kchem^1 \cdot e^{-\alpha \cdot \Phi_1} \cdot 1 \cdot L_1}{(50 \cdot \pi)^{0.5}}}$$

$$\Psi 1_k := \frac{\dfrac{Ket \cdot e^{-\alpha \cdot \Phi_k}}{(50 \cdot \pi)^{0.5}} + \dfrac{Kchem^1 \cdot e^{-\alpha \cdot \Phi_k} \cdot 1}{(1)^{0.5}} \cdot \displaystyle\sum_{j=1}^{k-1} \left(\Psi 1_j \cdot L_{k-j+1}\right) - 2Ket \cdot e^{-\alpha \cdot \Phi_k} \cdot \dfrac{\left(1 + e^{\Phi_k}\right)}{(50 \cdot \pi)^{0.5}} \cdot \displaystyle\sum_{j=1}^{k-1} \left(\Psi 1_j \cdot S_{k-j+1}\right)}{1 + \dfrac{2Ket \cdot e^{-\alpha \cdot \Phi_k} \cdot \left(1 + e^{\Phi_k}\right) \cdot S_1}{(50 \cdot \pi)^{0.5}} - \dfrac{Kchem^1 \cdot e^{-\alpha \cdot \Phi_k} \cdot 1 \cdot L_1}{(1)^{0.5}}}$$

$$p := 1 .. \left(\frac{\Delta E}{dE}\right) - 1$$

$$\Psi 1f_p := \Psi 1_{(p+1) \cdot 50} \qquad \Psi 1b_p := \Psi 1_{50 \cdot p + 25} \qquad \Psi 1net_p := \Psi 1f_p - \Psi 1b_p$$

$$E_p := Es - p \cdot dE$$



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