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Supplementary Materials

Irreversible Inactivation of Initial Form of Water-Soluble Redox Proteins-Theoretical Study in Square-Wave Voltammetry

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

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

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

$D := 0.000005$

$kc := 30055.2500$

$f := 10$

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

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

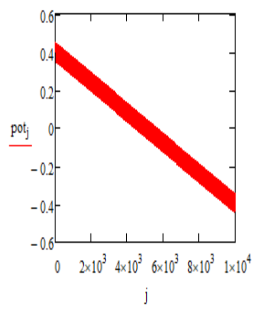
$\alpha := 0.5$

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

$Ket := \frac{ks}{f^{0.5} \cdot D^{0.5}} \qquad Ket = 100.002$

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

$Kchem = 3.006 \times 10^3$



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

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

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

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

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

$$\Psi1_1 := \frac{\frac{Ket\cdot e^{-\alpha\cdot\Phi_1}}{(50\cdot\pi)^{0.5}} - \left[2Ket\cdot e^{-\alpha\cdot\Phi_1}\cdot\frac{\left(1+e^{\Phi_1}\right)}{(50\cdot\pi)^{0.5}}\cdot 0 + \frac{Kchem^1\cdot e^{-\alpha\cdot\Phi_1}\cdot 1\cdot L_1}{(50\cdot\pi)^{0.5}}\right]}{1+\frac{2Ket\cdot e^{-\alpha\cdot\Phi_1}\cdot\left(1+e^{\Phi_1}\right)\cdot S_1}{(50\cdot\pi)^{0.5}} - \frac{Kchem^1\cdot e^{-\alpha\cdot\Phi_1}\cdot 1\cdot L_1}{(50\cdot\pi)^{0.5}}}$$

$$\Psi1_k := \frac{\frac{Ket\cdot e^{-\alpha\cdot\Phi_k}}{(50\cdot\pi)^{0.5}} + \frac{Kchem^1\cdot e^{-\alpha\cdot\Phi_k}\cdot 1}{(1)^{0.5}}\cdot\sum_{j=1}^{k-1}\left(\Psi1_j\cdot L_{k-j+1}\right) - 2Ket\cdot e^{-\alpha\cdot\Phi_k}\cdot\frac{\left(1+e^{\Phi_k}\right)}{(50\cdot\pi)^{0.5}}\cdot\sum_{j=1}^{k-1}\left(\Psi1_j\cdot S_{k-j+1}\right)}{1+\frac{2Ket\cdot e^{-\alpha\cdot\Phi_k}\cdot\left(1+e^{\Phi_k}\right)\cdot S_1}{(50\cdot\pi)^{0.5}} - \frac{Kchem^1\cdot e^{-\alpha\cdot\Phi_k}\cdot 1\cdot L_1}{(1)^{0.5}}}$$

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

$$\Psi1f_p := \Psi1_{(p+1)\cdot 50} \qquad \Psi1b_p := \Psi1_{50\cdot p+25} \qquad \Psi1net_p := \Psi1f_p - \Psi1b_p$$

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