

Supplementary Material

MATCAD File

IRREVERSIBLE INACTIVATION OF THE INITIAL REDOX FORM IN SURFACE ELECTRODE MECHANISM: THEORETICAL ASPECTS IN SQUARE-WAVE VOLTAMMETRY

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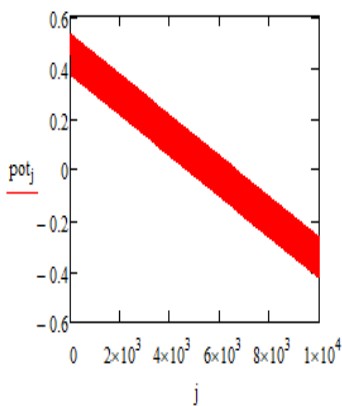
$$E_s := 0.45 \quad \Delta E := 0.8 \quad dE := 0.004 \quad E_{sw} := 0.08$$

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

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

$$\alpha := 0.5$$

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



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

$$S_k := e^{\frac{K_{chem}}{50} \cdot (-k)} - e^{\frac{K_{chem}}{50} \cdot (-k+1)}$$

$$\Phi_j := n \cdot \frac{F}{R \cdot T} \cdot pot_j \quad Ket := 0.032$$

$$k_c := 1000.00$$

$$f := 10$$

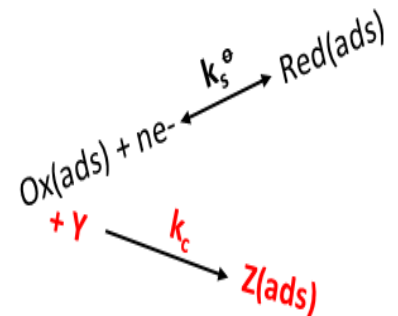
$$k_s := 10^{-0.5}$$

$$Ket := \frac{k_s}{f}$$

$$k_c := 10^3$$

$$K_{chem} := \frac{k_c}{f}$$

Model of Surface Electrode Mechanism
with Irreversible Chemical Reaction
Coupled to Initial Redox Form in
Protein-Film Voltammetry



Definitions and Meanings of the Symbols

f is the SW frequency
k_s is standard rate constant of electron transfer
α is electron transfer coefficient
n is number of exchanged electrons
dE is potential step
E_{sw} is square-wave amplitude
T is thermodynamic temperature
R is universal gas constant
k_c is rate constant of irreversible chemical reaction
K_{chem} is dimensionless kinetic chemical parameter
S_k is numerical integration factor
E_s is starting potential
Φ is dimensionless potentials
F is the Faraday constant
Ψ is dimensionless current

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$$\Psi_{1_1} := \frac{\frac{Ket}{50} \cdot e^{-\alpha \cdot \Phi_1} - \left[Ket \cdot e^{-\alpha \cdot \Phi_1} \cdot \frac{(1 + e^{\Phi_1})}{50} \cdot 0 + \frac{Kchem^1 \cdot e^{-\alpha \cdot \Phi_1} \cdot 1 \cdot S_1}{1} \right]}{1 + \frac{Ket \cdot e^{-\alpha \cdot \Phi_1} \cdot (1 + e^{\Phi_1})}{50} - \frac{Kchem^1 \cdot e^{-\alpha \cdot \Phi_1} \cdot 1 \cdot S_1}{1}}$$

$$\Psi_{1_k} := \frac{\frac{Ket}{50} \cdot e^{-\alpha \cdot \Phi_k} + \frac{Kchem^1 \cdot e^{-\alpha \cdot \Phi_k} \cdot 1}{1} \cdot \sum_{j=1}^{k-1} (\Psi_{1_j} \cdot S_{k-j+1}) - Ket \cdot e^{-\alpha \cdot \Phi_k} \cdot \frac{(1 + e^{\Phi_k})}{50} \cdot \sum_{j=1}^{k-1} \Psi_{1_j}}{1 + \frac{Ket \cdot e^{-\alpha \cdot \Phi_k} \cdot (1 + e^{\Phi_k})}{50} - \frac{Kchem^1 \cdot e^{-\alpha \cdot \Phi_k} \cdot 1 \cdot S_1}{1}}$$

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

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

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

