MATHCAD FILE FOR SIMULATION OF SIMPLE SURFACE Ox(ads) + ne- = Red(ads) Mechanism in Protein-Film Square-wave Voltammetry

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Abstract

Surface reaction Ox(ads) + ne- = Red(ads), in which both participants are firmly adsorbed at the working electrode surface is considered as an adequate model fpr many redox proteins analyzed in protein-film voltammetry. We give the readers entire working MATHCAD file to simulate this mechanism under conditions of square-wave voltammetry. The features of simulated voltammograms is function of number of exchanged electrons, electron transfer coefficient, potential step, square-wave amplitude, and on dimensionless parameter related to the kinetic of electron transfer, defined as λ = ks/f, where ks is standard rate constant of electron traansfer and ‘f’ is the SW frequency.

SIMPLE SURFACE MECHANISM
with both Ox and Red adsorbed
Ox(ads) +ne- = Red(ads)
λ is dimensionless kinetic parameter related to electron transfer step defined as λ = ks/f
ΔE is step potential
Esw is square-wave amplitude
Φ is dimensionless potential
k is counter
I is symbol of dimensionless current

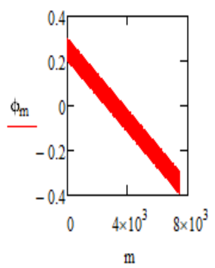
$Es := 0.25$ $\qquad \Delta E := 0.004 \quad Esw := 0.05$

$$m := 1 .. \frac{0.6}{\Delta E} \cdot 50$$

$$relativenpot_m := \left[\left(\mathrm{ceil}\left(\frac{m}{25} \cdot \frac{1}{2}\right) \cdot \Delta E + \mathrm{if}\left(\frac{\mathrm{ceil}\left(\frac{m}{25}\right)}{2} = \mathrm{ceil}\left(\frac{m}{25} \cdot \frac{1}{2}\right), 1, -1 \right) \cdot Esw + Esw \right) - \Delta E \right]$$

$$\phi_m := Es + Esw - relativenpot_m$$

$$\alpha := 0.5$$



$F := 96500 \quad n := 2 \quad R := 8.314 \quad T := 273.15 \quad i := 1..1$

$$\gamma_i := 10^{0.003 + i \cdot 0} \qquad \lambda_i := 10^{-1.5 \cdot i}$$

$$k := 1 .. \frac{0.6}{\Delta E} \cdot 50 \qquad M_{k,i} := e^{-\frac{\gamma_i}{50} \cdot (k-1)} - e^{-\frac{\gamma_i}{50} \cdot (k)}$$

$\log(\gamma_i) =$ $3 \cdot 10^{-3}$

$\log(\lambda_i) =$ -1.5

$$\Phi_m := \frac{n \cdot F}{R \cdot T} \cdot \phi_m$$

$$I_{1,i} := \lambda_i \cdot e^{-\alpha \cdot \Phi_1} \left[1 + \lambda_i \cdot e^{-\alpha \cdot \Phi_1} \cdot \left(1 + e^{\Phi_1}\right) \cdot R^{-1} \right]^{-1}$$

$$I_{m,i} := \lambda_i \cdot e^{-\alpha \cdot \Phi_m} \left[1 - \left(1 + e^{\Phi_m}\right) \cdot R^{-1} \cdot \sum_{j=1}^{m-1} I_{j,i} \right] \left[1 + \lambda_i \cdot e^{-\alpha \cdot \Phi_m} \cdot \left(1 + e^{\Phi_m}\right) \cdot R^{-1} \right]^{-1}$$

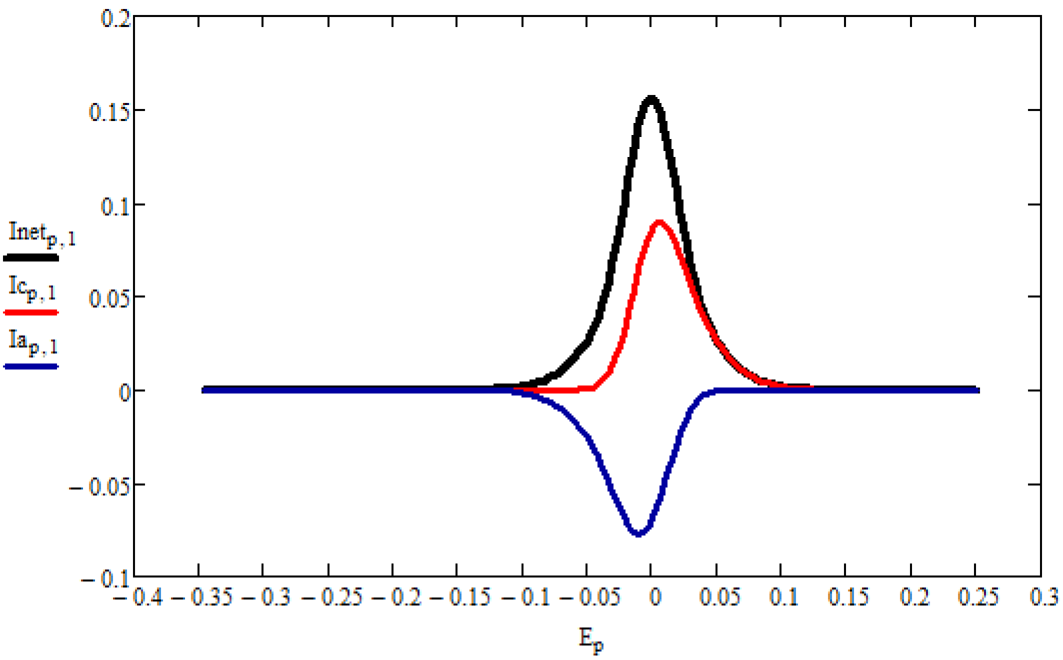
Povrsinska reakcija
SURFACE Mechanism
OX(ads) + ne = Red(ads)

$-\alpha \cdot \Phi_1$

$$p := 0..\frac{0.6}{\Delta E} - 1 \quad E_p := Es - p \cdot \Delta E$$

$$Ia_{p,i} := I_{50 \cdot p+25,i} \quad Ic_{p,i} := I_{(p+1) \cdot 50,i} \quad Inet_{p,i} := Ic_{p,i} - Ia_{p,i}$$

$$\Psi a_{p,i} := \Psi_{50 \cdot p+25,i} \quad \Psi c_{p,i} := \Psi_{(p+1) \cdot 50,i} \quad \Psi net_{p,i} := \Psi c_{p,i} - \Psi a_{p,i}$$



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