Protein Film Voltammetry of Two-Step Electrode Mechanism Associated with Intermediate Regenerative Reaction-MATHCAD Simulation Protocol

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$EsI := 0.25 \quad \Delta E := 1 \quad dE := 0.01 \quad Esw := 0.05 \quad EsII := 0.45$

$n := 1 \quad F := 96500 \quad R := 8.314 \quad T := 298.15 \quad \alpha := 0.5$

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

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

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

$k := 1 .. 1$

$ks1 := 10$

$ks2 := 10.000000000010$

$f := 10$

$$KI := \frac{ks1}{f}$$

$K := 00.00011$

K e konstanta na brzina na regenerativna reakcija

$$KII := \frac{ks2}{f}$$

$$\lambda := \frac{K}{f}$$

ks [s-1]
K [s-1]

λ e hemiski parametar

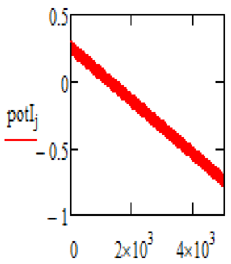
SURCACE ECatE
in SWV

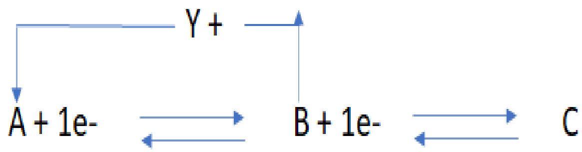
Model for two-step surface electrode mechanism associated with intermediate regenerative step

Erev – Erev

A + 1e=B + 1e-=C

B + Y – –› A





$$\Phi I_j := n \cdot \frac{F}{R \cdot T} \cdot potI_j \quad \Phi II_j := n \cdot \frac{F}{R \cdot T} \cdot potII_j$$

$$M_j := e^{-\lambda \cdot \frac{j}{50}} - e^{-\lambda \cdot \frac{j+1}{50}}$$

$x := 0.001$

$M_1 = 2.2 \times 10^{-7}$

$$\Psi I_1 := \frac{KI \cdot e^{-\alpha \cdot \Phi I_1}}{1 + \frac{KI \cdot \lambda^{-1} \cdot M_1}{1} \cdot e^{-\alpha \cdot \Phi I_1} + \frac{KI}{1} \lambda^{-1} \cdot e^{\Phi I_1 \cdot (1-\alpha)} \cdot M_1}$$

$\Psi I_1 = 3.697 \times 10^{-4}$

$M_2 = 2.2 \times 10^{-7}$

$x := 0.001$

$M_1 = 2.2 \times 10^{-7}$

$M_2 = 2.2 \times 10^{-7}$

$$\Psi I_1 := \frac{KI \cdot e^{-\alpha \cdot \Phi I_1}}{1 + \frac{KI \cdot \lambda^{-1} \cdot M_1}{1} \cdot e^{-\alpha \cdot \Phi I_1} + \frac{KI}{1} \lambda^{-1} \cdot e^{\Phi I_1 \cdot (1-\alpha)} \cdot M_1}$$

$\Psi I_1 = 3.697 \times 10^{-4}$

$$\Psi II_1 := \frac{\left(\Psi I_1 \cdot \frac{KII}{1} \cdot e^{-\alpha \cdot \Phi II_1}\right) - KII \cdot \frac{1}{1} \cdot e^{(1-\alpha) \cdot \Phi II_1} \cdot \Psi I_1 \cdot 1}{1 + \frac{KII \cdot e^{-\alpha \cdot \Phi II_1} \cdot 1}{1 \cdot 1} \cdot \left(1 + e^{\Phi II_1}\right)}$$

$\Psi II_1 = -3.697 \times 10^{-4}$

$x := 0.001$

Katalitcka povrsinska reakcija -kontrolen mehanizam

$$L_{1,i} := \frac{\lambda_i \cdot e^{-\alpha \cdot \Phi_1}}{1 + \lambda_i \cdot e^{-\alpha \cdot \Phi_1} \cdot \left(1 + e^{\Phi_1}\right) \cdot \frac{M_{1,i}}{\gamma_i}}$$

povrsinka kataliticka

$$\Psi I_j := \frac{\frac{KI}{1} \cdot e^{-\alpha \cdot \Phi I_j} - \frac{KI \cdot \lambda^{-1}}{1} \cdot e^{-\alpha \cdot \Phi I_j} \cdot \sum_{i=1}^{j-1} \left(\Psi I_i \cdot M_j\right) - \frac{KI}{1} \lambda^{-1} \cdot e^{\Phi I_j \cdot (1-\alpha)} \cdot \sum_{i=1}^{j-1} \left(\Psi I_i \cdot M_j\right)}{1 + \frac{KI \cdot \lambda^{-1} \cdot M_1}{1} \cdot e^{-\alpha \cdot \Phi I_j} + 1\lambda^{-1} \cdot e^{\Phi I_j \cdot (1-\alpha)} \cdot M_1}$$

$$L_{m,i} := \frac{\lambda_i \cdot e^{-\alpha \cdot \Phi_m} \cdot \left[1 - \frac{1 + e^{\Phi_m}}{\gamma_i} \cdot \sum_{j=1}^{m-1} \left[\Psi_{j,i} \cdot M_{(m-j)+1,i}\right]\right]}{1 + \lambda_i \cdot e^{-\alpha \cdot \Phi_m} \cdot \left(1 + e^{\Phi_m}\right) \cdot \frac{M_{1,i}}{\gamma_i}}$$

$$\Psi II_j := \frac{\frac{KII \cdot 1}{1} \cdot e^{-\alpha \cdot \Phi II_j} \cdot \sum_{i=1}^{j} \Psi I_i - KII1 \cdot e^{-\alpha \cdot \Phi II_j} \cdot \sum_{i=1}^{j-1} \left(\Psi II_i \cdot 1\right) - \frac{KII \cdot 1}{1} \cdot e^{(1-\alpha) \cdot \Phi II_j} \cdot (1) \cdot \sum_{i=1}^{j-1} \Psi II_i}{50 + \frac{KII \cdot 1}{1} \cdot e^{-\alpha \cdot \Phi II_j} \cdot \left(1 + e^{\Phi II_j}\right)}$$

$$z := 1$$

$$\phi I_j := z \cdot \frac{F}{R \cdot T} \cdot potI_j$$

$$II_1 := \frac{KI \cdot e^{-\alpha \cdot \phi I_1}}{1 + \frac{KI \cdot e^{-\alpha \cdot \phi I_1} \cdot \left(1 + e^{\phi I_1}\right)}{50}}$$

$$II_j := \frac{KI \cdot e^{-\alpha \cdot \phi I_j} - KI \cdot e^{-\alpha \cdot \phi I_j} \cdot \frac{\left(1 + e^{\phi I_j}\right)}{50} \cdot \sum_{i=1}^{j-1} II_i}{1 + \frac{KI \cdot e^{-\alpha \cdot \phi I_j} \cdot \left(1 + e^{\phi I_j}\right)}{50}}$$

$$\Psi_j := \Psi I_j + \Psi II_j$$

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

$$\Psi If_p := \Psi I_{(p+1) \cdot 50} \qquad \Psi Ib_p := \Psi I_{50 \cdot p+25} \qquad \Psi Inet_p := \Psi If_p - \Psi Ib_p$$

$$\Psi IIb_p := \Psi II_{50 \cdot p+25} \qquad \Psi IIf_p := \Psi II_{(p+1) \cdot 50} \qquad \Psi IInet_p := \Psi IIf_p - \Psi IIb_p$$

$$\Psi f_p := \Psi If_p + \Psi IIf_p$$

$$IIf_p := II_{(p+1) \cdot 50}$$

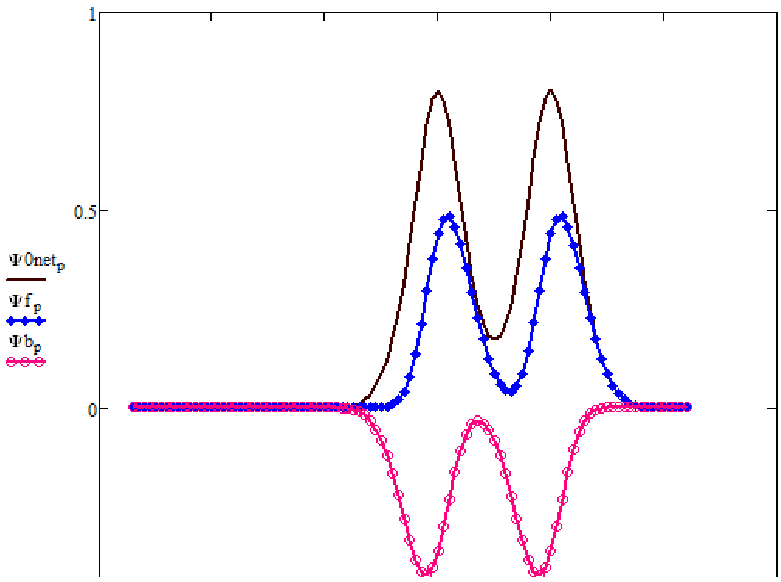
$$IIb_p := II_{50 \cdot p+25}$$

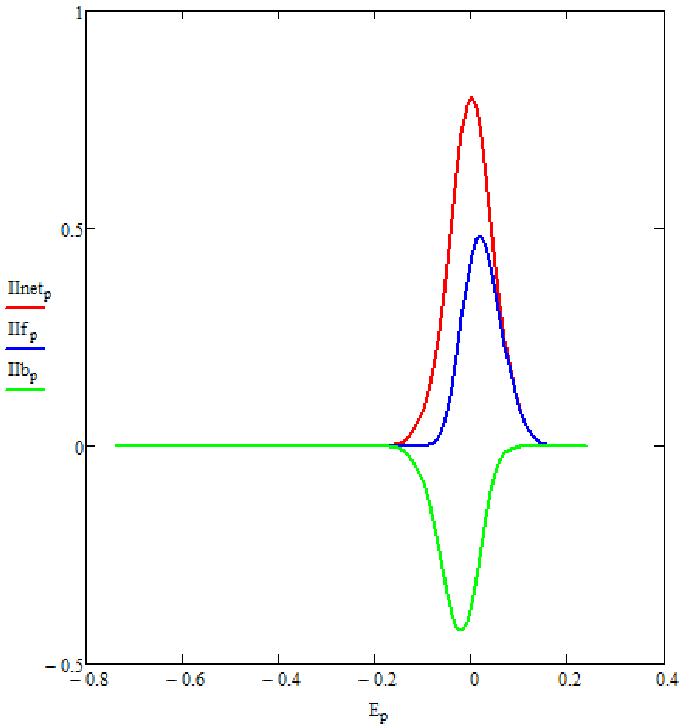
$$IInet_p := IIf_p - IIb_p$$

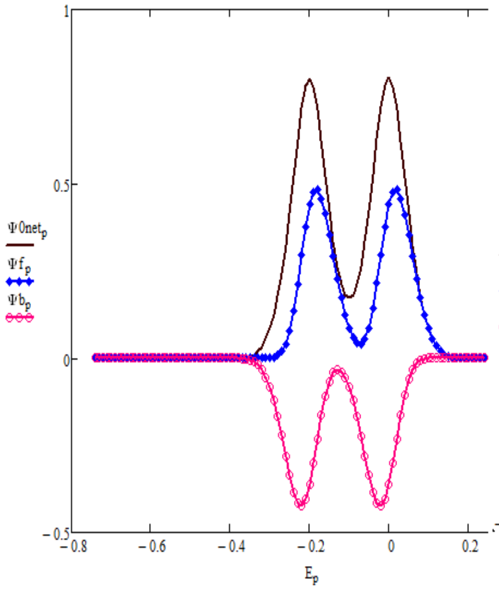
$$\Psi Ig_p := \Psi I_{50 \cdot p+14}$$

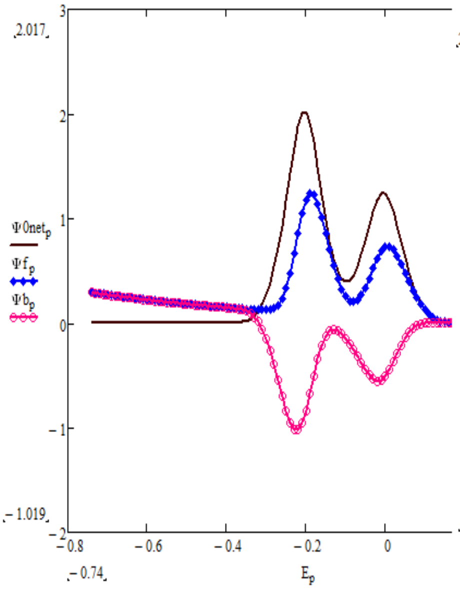
$$E_p := EsI - p \cdot dE \qquad \Psi b_p := \Psi Ib_p + \Psi IIb_p \qquad \Psi net_p := \Psi f_p - \Psi b_p$$

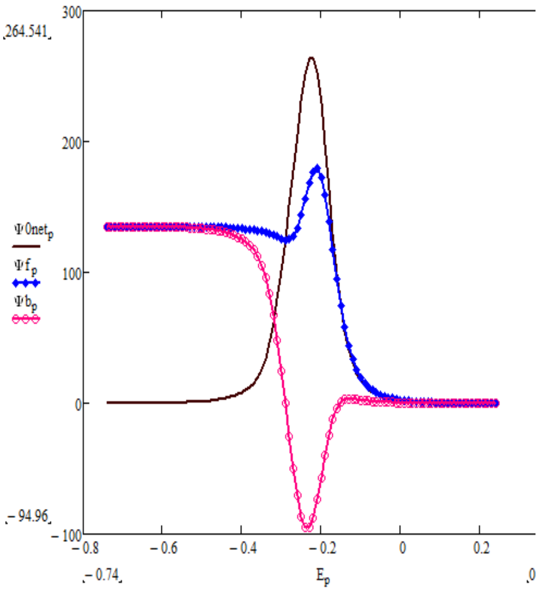
$$\Psi 0net_p := \Psi Inet_p + \Psi IInet_p$$

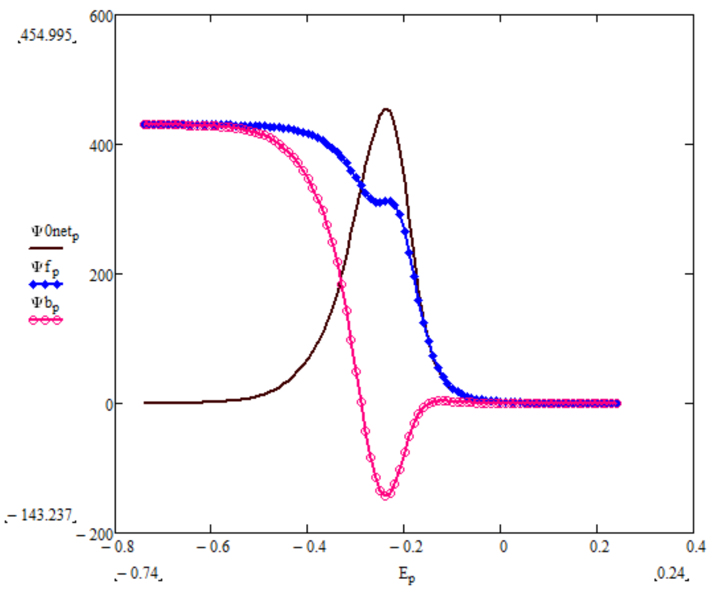


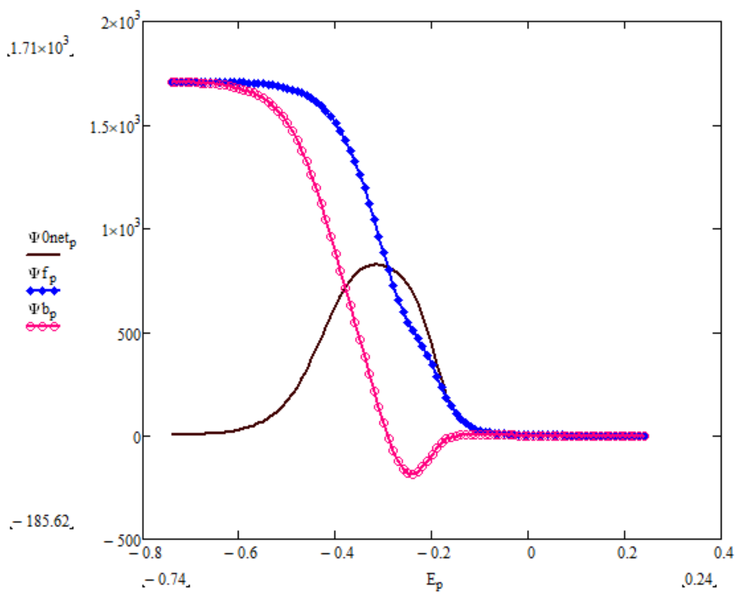



Ψ0net_p
Ψf_p
Ψb_p
E_p


2.017
Ψ0net_p
Ψf_p
Ψb_p
− 1.019
− 0.74
E_p


264.541
Ψ0net_p
Ψf_p
Ψb_p
− 94.96
− 0.74
E_p
0


454.995
Ψ0net_p
Ψf_p
Ψb_p
− 143.237
− 0.74
E_p
0.24


1.71×10^3
Ψ0net_p
Ψf_p
Ψb_p
− 185.62
− 0.74
E_p
0.24

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