MATHCAD FILE SURFACE EEC' CATALYTIC MECHANISM IN SQUARE-WAVE VOLTAMMETRY

THEORETICAL MODELLING OF A SURFACE EEC# CATAlyTIC MECHANISM in SWV MATHCAD FILE with all simulation parameters

KI and KII are electron transfer dimensionless parameters releated to the first and the second electron transfer steps

λ is catalytic parameter related to the kinetics of catalytic chemical step

k is rate constant of catalytic reaction

f is the SW frequency

M is numerical integration fatcor

$EsI := 0.3$ $\Delta E := 0.8$ $dE := 0.004$ $Esw := 0.05$ $k := 0.35$ $EsII := 0.3$

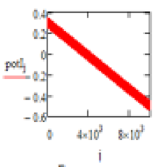
$n := 1$ $F := 96500$ $R := 8.314$ $T := 298.15$ $f := 10$ $\alpha := 0.5$ $ks1 := 2$ $ks2 := 2$

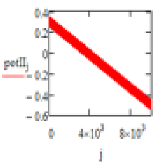
$j := 1 .. \frac{\Delta E}{dE} \cdot 50$

$KI := \frac{ks1}{f}$ $KII := \frac{ks2}{f}$ $\omega := \frac{k}{f}$ $\lambda := \frac{k}{f}$ $\gamma := \frac{k}{f}$

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

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





$\omega_1 = ▪$

$\log(\omega_1) = ▪$

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

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

$x := 0.001$

$$\Psi I_1 := root\left[x - KI \cdot e^{-\alpha \cdot \Phi I_1} + KI \cdot e^{-\alpha \cdot \Phi I_1} \cdot \left(1 + e^{\Phi I_1}\right) \cdot x - KI \cdot e^{\Phi I_1 \cdot (1-\alpha)} \cdot \frac{KII \cdot e^{-\alpha \cdot \Phi II_1} \cdot \frac{x \cdot M_1}{\gamma}}{50 \cdot \left[1 + KII \cdot e^{-\alpha \cdot \Phi II_1} \cdot \left(1 + e^{\Phi II_1}\right) \cdot \frac{M_1}{\gamma}\right]}, x\right]$$

$M_{1,c} =$ ▪

$$\Psi II_1 := \frac{\Psi I_1 \cdot \left(KII \cdot e^{-\alpha \cdot \Phi II_1}\right)}{50 \cdot \left[1 + KII \cdot e^{-\alpha \cdot \Phi II_1} \cdot \frac{\left(1 + e^{\Phi II_1}\right) \cdot M_1}{\gamma}\right]}$$

$\Psi I_1 = 1.265 \times 10^{-5}$ $\Psi II_1 = 0$ $x := 0.001$

$$\Psi I_j := root\left[x - KI \cdot e^{-\alpha \cdot \Phi I_j} + \frac{KI}{50} \cdot e^{-\alpha \cdot \Phi I_j} \cdot \left(1 + e^{\Phi I_j}\right) \cdot \left(x + \sum_{i=1}^{j-1} \Psi I_i\right) - KI \cdot e^{\Phi I_j \cdot (1-\alpha)} \cdot \left[\left[\frac{KII \cdot e^{-\alpha \cdot \Phi II_j} \cdot \left(x + \sum_{i=1}^{j-1} \Psi I_i\right)}{50 \cdot \left[1 + KII \cdot e^{-\alpha \cdot \Phi II_j} \cdot \left(1 + e^{\Phi II_j}\right) \cdot \frac{M_1}{\gamma}\right]} - KII \cdot e^{-\alpha \cdot \Phi II_j} \cdot \frac{\frac{1 + e^{\Phi II_j}}{\gamma}}{1 + KII \cdot e^{-\alpha \cdot \Phi II_j} \cdot \frac{M_1 \cdot \left(1 + e^{\Phi II_j}\right)}{\gamma}} \cdot \left[KII \cdot e^{\Phi II_j \cdot (1-\alpha)}\right]^{-1} \cdot \left[1 - KII \cdot e^{-\alpha \cdot \Phi II_j} + \frac{KII}{50} \cdot e^{-\alpha \cdot \Phi II_j} \cdot \left(1 + e^{\Phi II_j}\right) \cdot \left(x + \sum_{i=1}^{j-1} \Psi II_i\right)\right]\right] \ldots \right] \text{[illegible]}$$

$$\Psi II_j := \frac{KII \cdot e^{-\alpha \cdot \Phi II_j} \cdot \left(\sum_{i=1}^{j} \Psi I_i\right)}{50 \cdot \left[1 + KII \cdot e^{-\alpha \cdot \Phi II_j} \cdot \left(1 + e^{\Phi II_j}\right) \cdot \left(\frac{M_1}{\gamma}\right)\right]} - KII \cdot e^{-\alpha \cdot \Phi II_j} \cdot \frac{\frac{\left(1 + e^{\Phi II_j}\right)}{\gamma} \cdot \sum_{i=1}^{j-1} \left(\Psi II_i \cdot M_{j-i+1}\right)}{1 + KII \cdot e^{-\alpha \cdot \Phi II_j} \cdot \frac{M_1 \cdot \left(1 + e^{\Phi II_j}\right)}{\gamma}}$$

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

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

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

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

$$\Psi netb_p := \Psi Ib_p + \Psi IIb_p$$

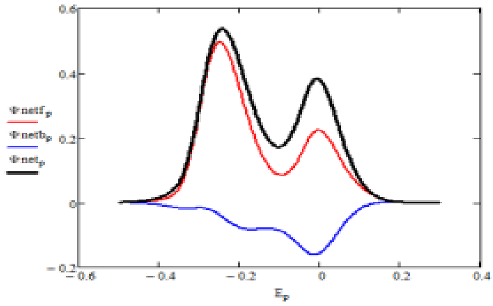
$$E_p := EsI - p\cdot dE$$

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

$KI := 1$

$KII := 1$

se zgolemuva kc-kataliticki parametar



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