EE Diffusional Mechanism in SWV-MATHCAD Simulation Protocol

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TWO STEP DIFFUSIONAL EE Mechanism in SWV--- this is EE diffusional mechanism with regenerative irreversible reaction associated with the product of first electrode transformation in which λ regenerative chemical parameter is very low

$EsI := 0.35 \quad \Delta E := 1.3 \quad dE := 0.01 \quad Esw := 0.05$

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

$EsII := 0.8 \quad r := 1..1$

$KI_r := 10^{.5 \cdot r}$

$KII := 10^{.5}$

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

$\alpha 2 := 0.5$

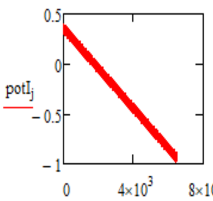
$\alpha 1 := 0.5 \quad \log(KI_r) = \boxed{0.5}$

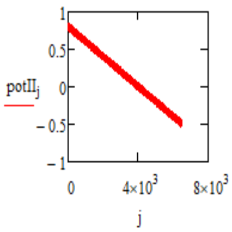
$\lambda := .0001235$

$KI_1 = 3.162$

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

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





$$M1_j := \sqrt{\frac{j}{1}} - \sqrt{\frac{j-1}{1}}$$

$$A_j := \left(1 - erfc\left(\sqrt{\frac{\lambda}{50 \times 1}\cdot j}\right)\right) - \left[1 - erfc\left[\sqrt{\frac{\lambda}{50 \times 1}\cdot (j-1)}\right]\right]$$

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

$x := 0.001$

$$\Psi I_{1,r} := \frac{\frac{KI_r}{1}\cdot\frac{2}{\sqrt{4}}\cdot e^{-\alpha 1\cdot\Phi I_1} - 0}{1 + \frac{KI_r\cdot\lambda^{-1}\cdot A_1}{\frac{2}{\sqrt{4}}}\cdot e^{-\alpha 1\cdot\Phi I_1} + 1\lambda^{-1}\cdot e^{\Phi I_1\cdot(1-\alpha 1)}\cdot A_1\cdot\frac{\frac{1}{\sqrt{4}}}{2}}$$

$$\Psi II_{1,r} := \frac{\frac{2}{\sqrt{\pi\cdot 50}}KII\cdot e^{-\alpha 2\cdot\Phi II_1}}{1 + \frac{KII\cdot M1_1\cdot 2}{\sqrt{\pi\cdot 50}}\cdot e^{-\alpha 2\cdot\Phi II_1}\cdot\left(1 + e^{\Phi II_1}\right)}\cdot\Psi I_{1,r}\cdot A_1 + \frac{KII\cdot e^{-\alpha 2\cdot\Phi II_1}}{1 + \frac{2\cdot KII\cdot M1_1\cdot e^{-\alpha 2\cdot\Phi II_1}}{\sqrt{\pi\cdot 50}} + \frac{2\cdot KII\cdot e^{(1-\alpha 2)\cdot\Phi II_1}}{\sqrt{\pi\cdot 50}}\cdot 1}\cdot 1$$

$\Psi I_{1,1} = 3.802 \times 10^{-8}$

$\Psi II_{1,1} = 2.667 \times 10^{-14}$

$$\Psi I_{j,r} := \frac{\frac{KI_r}{\sqrt{4}} \cdot 2 \cdot e^{-\alpha 1 \cdot \Phi I_j} - \frac{KI_r \cdot \lambda^{-1} \cdot \frac{2}{\sqrt{4}}}{1} \cdot e^{-\alpha 1 \cdot \Phi I_j} \cdot \sum_{i=1}^{j-1} \left(\Psi I_{i,r} \cdot A_{j-i+1}\right) - \frac{KI_r}{1} \lambda^{-1} \cdot \frac{2}{\sqrt{4}} \cdot e^{\Phi I_j \cdot (1-\alpha 1)} \cdot \sum_{i=1}^{j-1} \left(\Psi I_{i,r} \cdot A_{j-i+1}\right)}{1 + \frac{KI_r \cdot \lambda^{-1} \cdot A_1 \cdot 2}{\sqrt{4}} \cdot e^{-\alpha 1 \cdot \Phi I_j} + 1\lambda^{-1} \cdot e^{\Phi I_j \cdot (1-\alpha 1)} \cdot A_1 \cdot \frac{2 \cdot KI_r}{\sqrt{4}}}$$

$$\Psi II_{j,r} := \frac{\frac{\frac{2}{\sqrt{\pi \cdot 50}} KII \cdot e^{-\alpha 2 \cdot \Phi II_j}}{1+0} \cdot \sum_{i=1}^{j} \left(\Psi I_{i,r} \cdot M1_{j-i+1}\right) - KII \frac{2}{\sqrt{\pi \cdot 50}} \cdot e^{-\alpha 2 \cdot \Phi II_j} \cdot \sum_{i=1}^{j-1} \left(\Psi II_{i,r} \cdot M1_{j-i+1}\right) - \frac{2}{\sqrt{\pi \cdot 50}} KII \cdot e^{1 \cdot \Phi II_j \cdot (1-\alpha 2)} \cdot (1) \cdot \sum_{i=1}^{j-1} \left(\Psi II_{i,r} \cdot M1_{j-i+1}\right)}{1 + \frac{KII \cdot \frac{2 \cdot M1_1}{\sqrt{\pi \cdot 50}}}{1} \cdot e^{-\alpha 2 \cdot \Phi II_j} \cdot \left(1 + e^{\Phi II_j}\right)}$$

$\Psi_{j,r} := \Psi I_{j,r} + \Psi II_{j,r}$

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

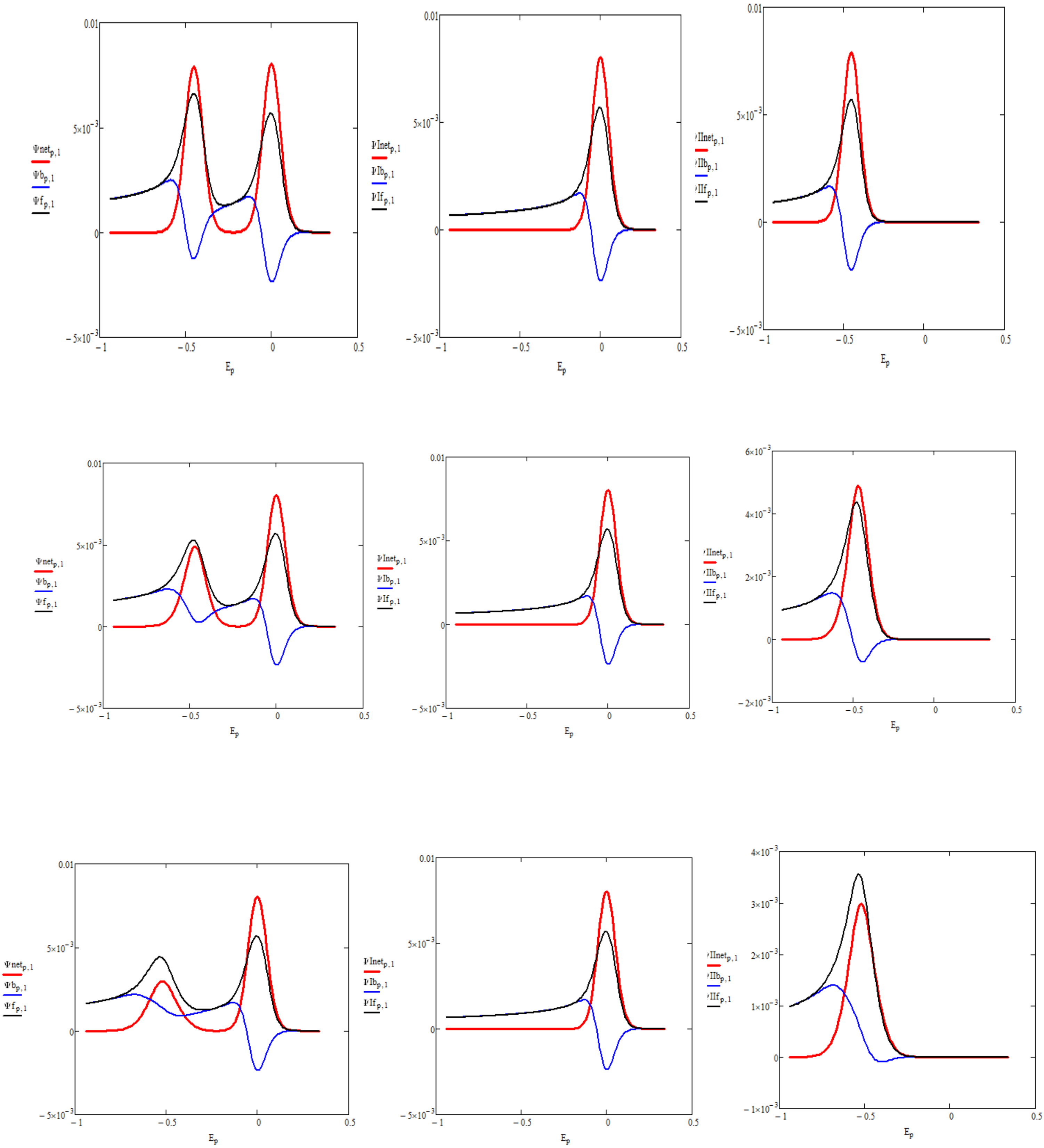
$\Psi If_{p,r} := \Psi I_{(p+1) \cdot 50,r}$ $\Psi Ib_{p,r} := \Psi I_{50 \cdot p+2}$ $\Psi Inet_{p,r} := \Psi If_{p,r} - \Psi Ib_{p,r}$

$\Psi IIb_{p,r} := \Psi II_{50 \cdot p+25,r}$ $\Psi IIf_{p,r} := \Psi II_{(p+1)}$ $\Psi IInet_{p,r} := \Psi IIf_{p,r} - \Psi IIb_{p,r}$

$E_p := EsI - p \cdot dE$

$\Psi b_{p,r} := \Psi_{50 \cdot p+25,r}$ $\Psi f_{p,r} := \Psi_{(p+1) \cdot 5(}$ $\Psi net_{p,r} := \Psi f_{p,r} - \Psi b_{p,r}$

Effect of Different kinetics of First and Second Electron transfer Step to the Features of Simulated Square-wave Voltammograms



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