Влијание на кинетиката на регенеративната хемиска реакција поврзана со првата електродна трансформација врз квадратно-брановите волтаметриски одговори на на EC'EC' површински регенеративен механизам во услови на значителна кинетика на двата електродни чекори

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Abstract: Претсавен е MATHCAD протокол за двостепени површински електроден механизам поврзан со две последователни регенеративни хемиски реакции, во услови на квадратно-бранова волтаметрија. За прв пат овој механизам овозможува симулирање на однесувањето на липофилни редокс ензими, чија електрохемиска трансформација се одвива во два последователни чекори. Фајлот е достапен во слободна форма и е достапен за симулирање со аплицирање во MATHCAD симулацискиот пакет.

TWO STEP SURFACE EC'EC'cat Mechanism in SWV—new version 12 04 2024 OK-Effect of catalysis of first step in both KI and KII different values

$EsI := 0.25 \quad \Delta E := 1 \quad dE := 0.01 \quad Esw := 0.065 \quad EsII := 0.55 \quad r := 1..1$

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

$KI_r := 10^{1 \cdot r}$

$KII := 10^1$

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

$\alpha 2 := 0.5 \quad \alpha 1 := 0.5 \quad \log(KI_r) =$

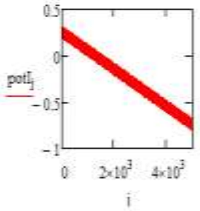
$\lambda := .004600600006100$

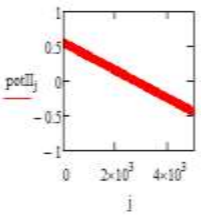
λ e kineticki parametar na regenerativna hemiska reakcija povrzana so prv elektroden cekor

$KI_1 = 10$

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

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





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

$z := .000000610$

z e kataliticki regenerativen hemiski parametar povrzan so vtor cekor

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

$$B_j := e^{-z \cdot \frac{j}{50}} - e^{-z \cdot \frac{j+1}{50}}$$

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

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

$\Psi I_{1,1} = 2.131 \times 10^{-3}$

$\Psi II_{1,1} = 0$

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

$$\Psi II_{j,r} := \frac{KII\,\frac{1}{\lambda}\cdot e^{-\alpha 2\cdot\Phi II_j}\cdot\sum_{i=1}^{j}\left(\Psi I_{i,r}\cdot A_{j-i+1}\right) - \frac{1}{(z)}KII\cdot e^{\Phi II_j\cdot(-\alpha 2)}\cdot\sum_{i=1}^{j-1}\left(\Psi II_{i,r}\cdot B_{j-i+1}\right) - \frac{1}{(z)}KII\cdot e^{1\cdot\Phi II_j\cdot(1-\alpha 2)}\cdot\sum_{i=1}^{j-1}\left(\Psi II_{i,r}\cdot B_{j-i+1}\right)}{1 + \frac{1\cdot B_1}{(z)}KII\cdot e^{\Phi II_j\cdot(-\alpha 2)} + \frac{1\cdot B_1}{(z)}KII\cdot e^{\Phi II_j\cdot(1-\alpha 2)}}$$

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

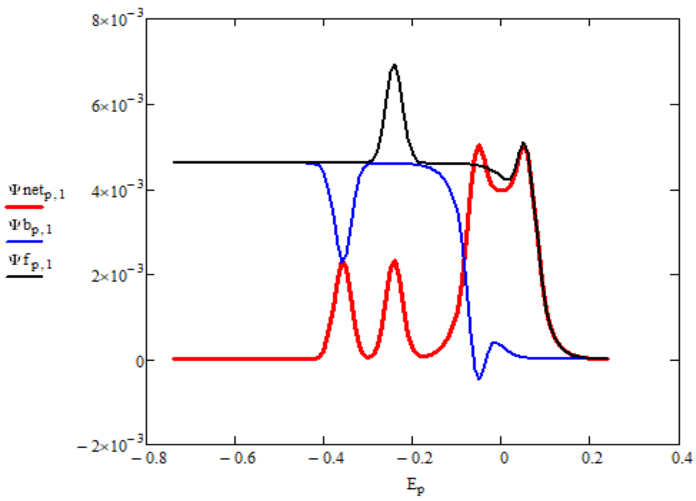
$$p := 1..\left(\frac{\Delta E}{dE}\right) - 1$$

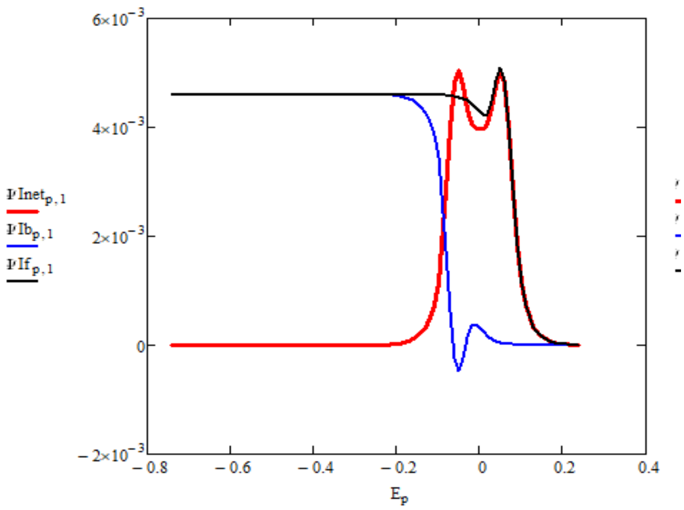
$\Psi If_{p,r} := \Psi I_{(p+1)\cdot 50,r}$ $\Psi Ib_{p,r} := \Psi I_{50\cdot p+2}$ $\Psi Inet_{p,r} := \Psi If_{p,r} - \Psi Ib_{p,r}$

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

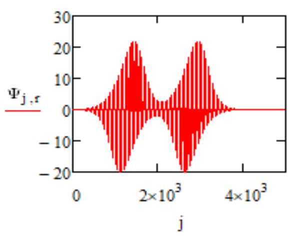
$E_p := EsI - p\cdot dE$

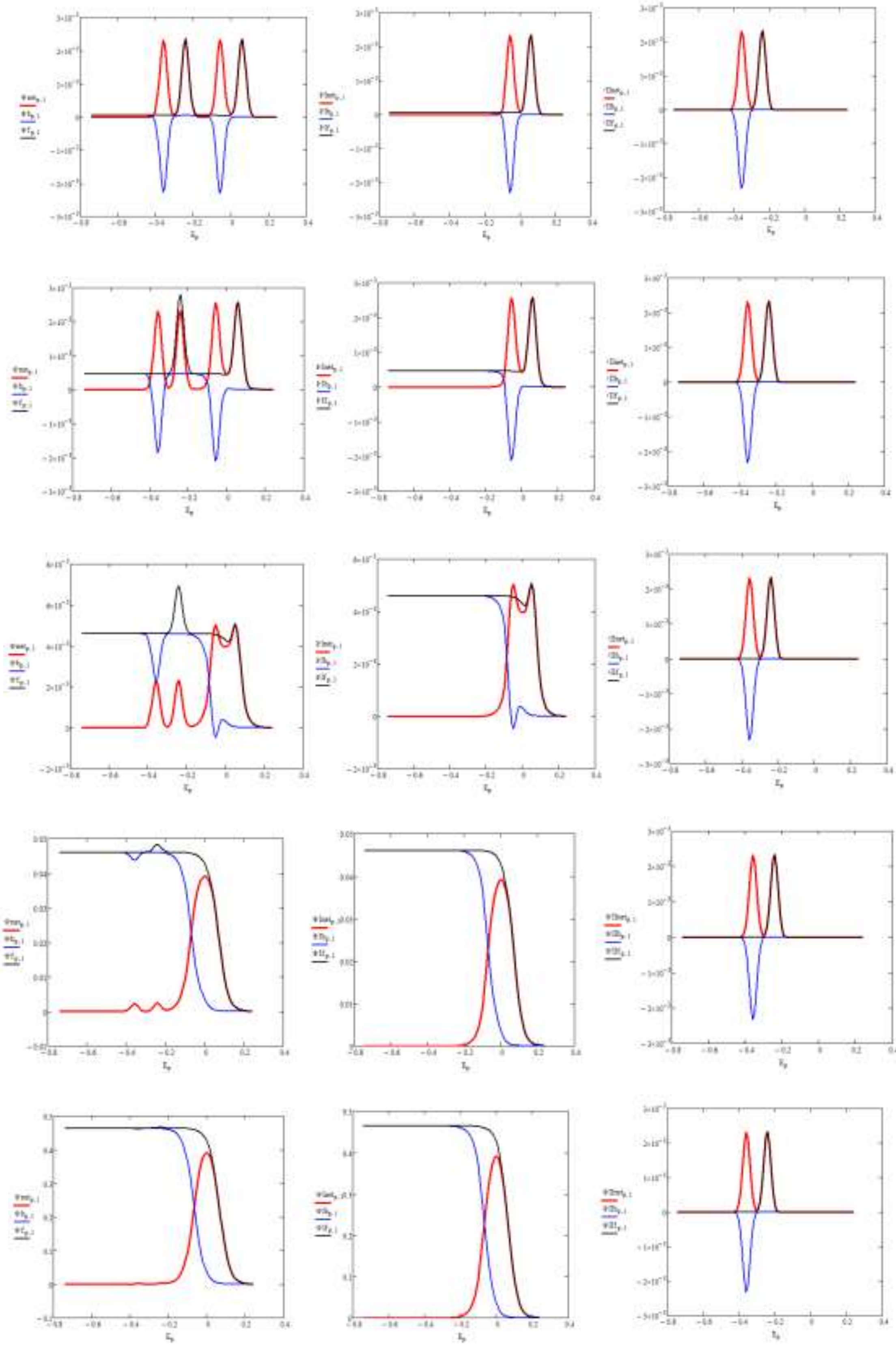
$\Psi b_{p,r} := \Psi_{50\cdot p+25,r}$ $\Psi f_{p,r} := \Psi_{(p+1)\cdot 5(}$ $\Psi net_{p,r} := \Psi f_{p,r} - \Psi b_{p,r}$





$\Psi f_{p,1} =$ $\Psi b_{p,1} =$ $\Psi net_{p,1} =$





Влијание на константата на регенеративна хемиска реакција Поврзана со првата електродна трансформација врз квадратно-брановите волтаметриски одговори на EC’EC’ механизам симулирани во услови на големи брзини на константите на трансфер на електрони на двата електродни чекори

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