Supplementary Material-a MATHCAD SIMULATION FILE WITH ALL PARAMETERS FOR CALCULATING SQUARE-WAVE VOLTAMMOGRAMS related to paper:
V. Mirčeski and **R. Gulaboski**, “A Theoretical and Experimental Study of Two-Step Quasireversible Surface Reaction by Square-Wave Voltammetry” ***Croat. Chem. Acta*** 76 (2003) 37-48.

Square-wave voltammetry of surface TWO-STEP protein film voltammetry
Valentin Mirceski, Rubin Gulaboski

$EsI := 0.2$ $\quad \Delta E := 0.8$ $\quad dE := 0.01$ $\quad Esw := 0.05$ $\quad EsII := 0.6$ $\quad r := 1..1$

$n := 1$ $\quad F := 96500$ $\quad R := 8.314$ $\quad T := 298.15$ $\quad KI_r := 10^{.8 \cdot r}$

$KII := 10^{.75}$

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

$\alpha 2 := 0.5$

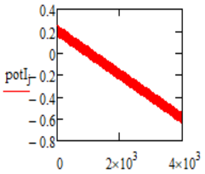
$\alpha 1 := 0.5$ $\quad \log(KI_r) = \boxed{0.8}$

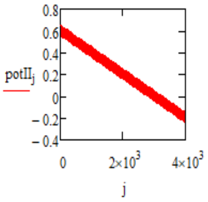
$$potI_j := EsI + Esw - \left[\left(ceil\left(\frac{j}{25} \cdot \frac{1}{2}\right) \cdot dE + if\left(\frac{ceil\left(\frac{j}{25}\right)}{2} = ceil\left(\frac{j}{25} \cdot \frac{1}{2}\right), 1, -1\right) \cdot Esw + Esw\right) - dE\right]$$

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

TWO STEP SURFACE EE MECHANISM
PROTEIN FILM VOLTAMMETRY IN
SQUARE WAVE VOLTAMMETRY

KI and KII are kinetic parameters related to the first and second electron transfer step
alpha is the electron transfer coefficient
EsI and EsII are potentials related to the first and the second electron transfer step
n is number of electron exchanged
F is Faraday constant
Esw is SWV amplitude
T is temperature
dE is potential step
Φ is dimensionless potential
Ψ is dimensionless current





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

$x := 0.001$

$$\Psi I_{1,r} := \mathrm{root}\left[\left[1+\frac{KI_r\cdot e^{-\alpha1\cdot\Phi I_1}}{50}\cdot\left(1+e^{\Phi I_1}\right)\right]\cdot x-\frac{KI_r}{50}\cdot e^{(1-\alpha1)\cdot\Phi I_1}\cdot\left[\frac{x\cdot\frac{KII\cdot e^{-\alpha2\cdot\Phi II_1}}{50}}{1+\frac{KII\cdot e^{-\alpha2\cdot\Phi II_1}}{50}\cdot\left(1+e^{\Phi II_1}\right)}\right]-KI_r\cdot e^{-\alpha2\cdot\Phi I_1},x\right]$$

$$\Psi II_{1,r} := \frac{\Psi I_{1,r}\cdot\frac{KII\cdot e^{-\alpha2\cdot\Phi II_1}}{50}}{1+\frac{KII\cdot e^{-\alpha2\cdot\Phi II_1}}{50}\cdot\left(1+e^{\Phi II_1}\right)}$$

$\Psi I_{1,1} = 2.796\times10^{-3}$ $\Psi II_{1,3} =$ ▮

$x := 0.001$

$$\Psi I_{j,r} := \mathrm{root}\Bigg[x-KI_r\cdot e^{-\alpha1\cdot\Phi I_j}\cdot\Bigg[1-\Bigg[\frac{1}{50}\cdot\left(1+e^{\Phi I_j}\right)\cdot\left(x+\sum_{i=1}^{j-1}\Psi I_{i,r}\right)+\frac{e^{\Phi I_j}}{50}\cdot\Bigg[\frac{1}{1+e^{\Phi II_j}}\cdot\left(x+\sum_{i=1}^{j-1}\Psi I_{i,r}\right)-\frac{50}{KII\cdot e^{-\alpha2\cdot\Phi II_j}\cdot\left(1+e^{\Phi II_j}\right)}\cdot\Bigg[KII\cdot e^{-\alpha2\cdot\Phi II_j}\cdot\Bigg[\frac{1}{50}\cdot\left(x+\sum_{i=1}^{j-1}\Psi I_{i,r}\right)-\frac{1}{50}\cdot\left(1+e^{\Phi II_j}\right)\cdot\Bigg[\frac{50\cdot x}{KI_r\cdot e^{(1-\alpha1)\cdot\Phi I_j}}-50\cdot e^{-\Phi I_j}\cdot\Bigg[1-\frac{1}{50}\cdot\left(1+e^{\Phi I_j}\right)\cdot\left(x+\sum_{i=1}^{j-1}\Psi I_{i,r}\right)\Bigg]\Bigg]\Bigg]\Bigg]\Bigg]\Bigg]\Bigg],x\Bigg]$$

$$\Psi II_{j,r} := \frac{KII\cdot e^{-\alpha2\cdot\Phi II_j}}{50+KII\cdot e^{-\alpha2\cdot\Phi II_j}\cdot\left(1+e^{\Phi II_j}\right)}\cdot\sum_{i=1}^{j}\Psi I_{i,r}-\frac{KII\cdot e^{(-\alpha2)\cdot\Phi II_j}\cdot\left(1+e^{\Phi II_j}\right)}{50+KII\cdot e^{-\alpha2\cdot\Phi II_j}\cdot\left(1+e^{\Phi II_j}\right)}\cdot\sum_{i=1}^{j-1}\Psi II_{i,r}$$

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

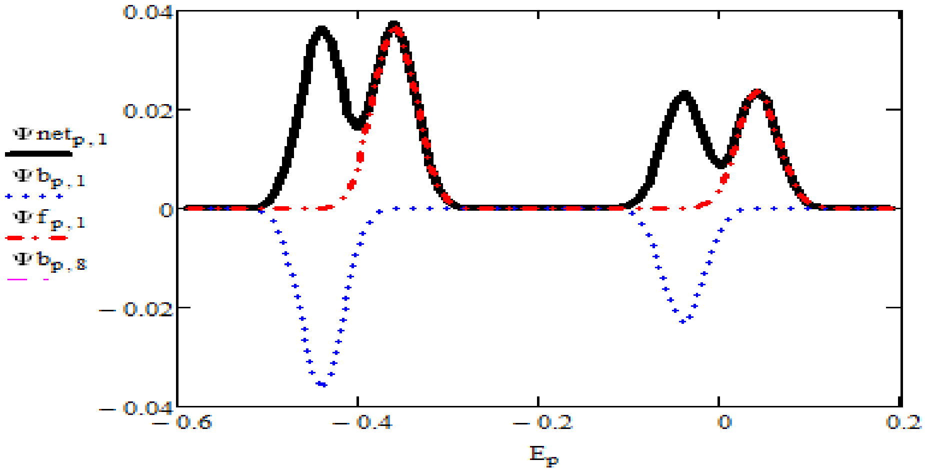
$p := 1 .. \left(\frac{\Delta E}{dE}\right) - 1$

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

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

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

$E_p := EsI - p\cdot dE$



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