EC’EC” Diffusional Mechanism with asymmetrical number of electrons in Square-wave Voltammetry

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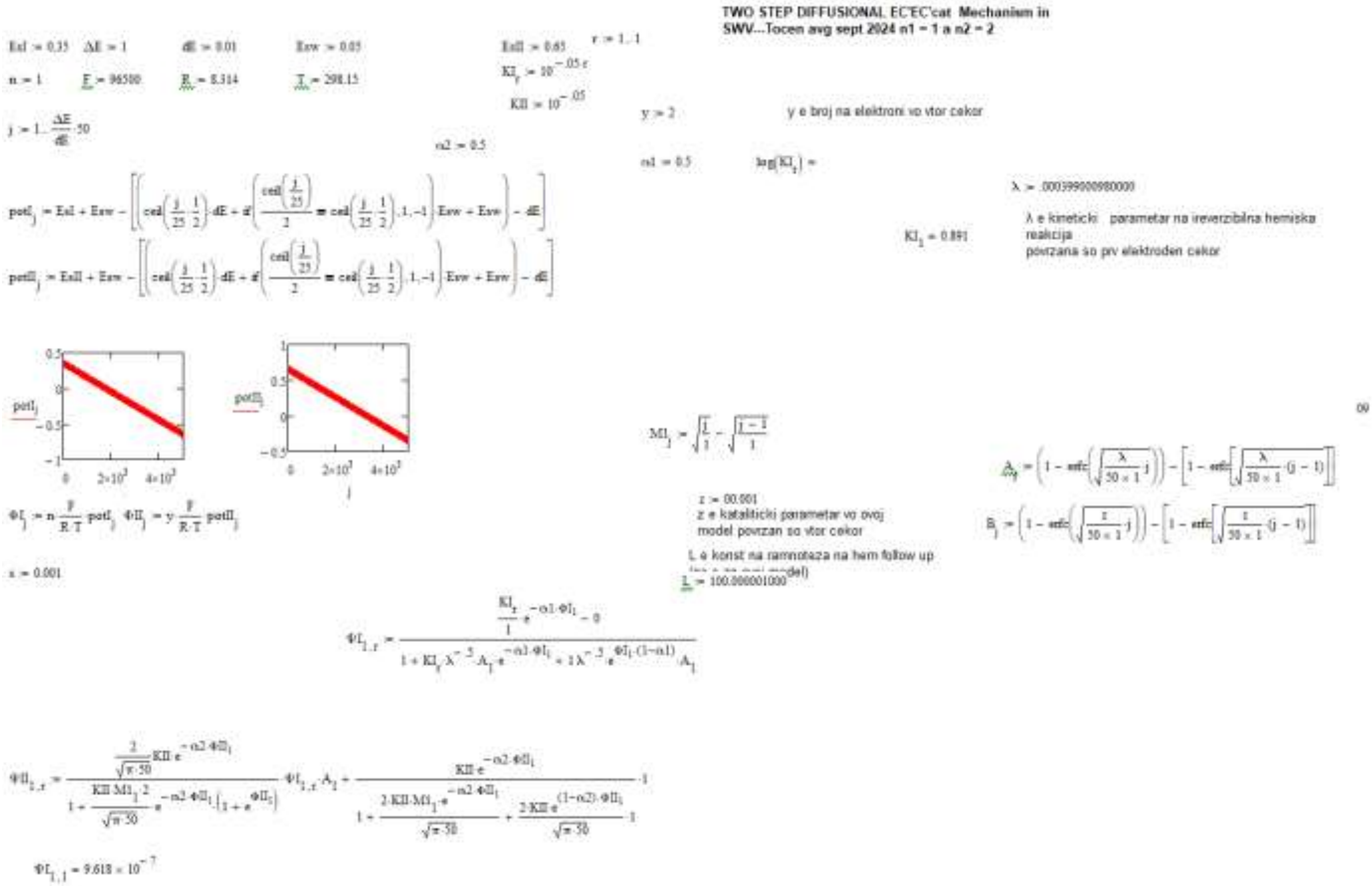
Abstract:

An on-line MATHCAD simulation platform for regenerative two step EC’EC’ mechanism, in which products of both electrons transfers are regenerated, is presented. Simulation protocol considers different number of electrons involved in both electron transfer steps. The platform is free to use for everyone. This models gives insights about the effect of number of exchanged electrons to the features of both peaks in scenario of nicely separated and completely overlapped electron transfer steps. It is very important mechanism that fits to the redox behavior of many redox enzymes under physiological conditions.



$$\Phi I_{j,r} = \frac{KI_r e^{-\alpha1 \cdot \Phi I_j} - KI_r \frac{1}{\sqrt{\lambda}} e^{-\alpha1 \cdot \Phi I_j} \sum_{i=1}^{j-1} \left(\Phi I_{i,r} \cdot A_{j-i+1}\right) - KI_r \lambda^{-0.5} e^{\Phi I_j (1-\alpha1)} \sum_{i=1}^{j-1} \left(\Phi I_{i,r} \cdot A_{j-i+1}\right)}{1 + KI_r \frac{2}{\sqrt{\lambda}} A_1 e^{-\alpha1 \cdot \Phi I_j} + \lambda^{-0.5} e^{\Phi I_j (1-\alpha1)} A_1 KI_r}$$

$$\Phi II_{j,r} = \frac{KII \frac{1}{\sqrt{\lambda}} e^{-\alpha2 \cdot \Phi II_j} \sum_{i=1}^{j} \left(\Phi I_{i,r} \cdot A_{j-i+1}\right) - KII \frac{0}{\sqrt{\lambda}} e^{(-\alpha2) \cdot \Phi II_j} \sum_{i=1}^{j} \left(\Phi I_{i,r} \cdot A_{j-i+1}\right) - \frac{0}{\sqrt{\pi \cdot 30}} \frac{KII}{1+0} e^{1 \cdot \Phi II_j (-\alpha2)} (1) \sum_{i=1}^{j-1} \left(\Phi II_{i,r} \cdot MI_{j-i+1}\right) - \frac{1}{(\sqrt{2}) \cdot (1+0)} KII e^{1 \cdot \Phi II_j (-\alpha2)} (1) \sum_{i=1}^{j-1} \left(\Phi II_{i,r} \cdot B_{j-i+1}\right) - \frac{1}{(\sqrt{2}) \cdot (1+0)} KII e^{1 \cdot \Phi II_j (1-\alpha2)} (1) \sum_{i=1}^{j-1} \left(\Phi II_{i,r} \cdot B_{j-i+1}\right)}{1 + KII \frac{A_1 \cdot 0}{\sqrt{\lambda}} e^{(-\alpha2) \cdot \Phi II_j} + \frac{0 MI_1}{\sqrt{\pi \cdot 30}} \frac{KII}{1+0} e^{1 \cdot \Phi II_j (-\alpha2)} + \frac{1 B_1}{(\sqrt{2}) \cdot (1+0)} KII e^{1 \cdot \Phi II_j (-\alpha2)} + \frac{1 B_1}{(\sqrt{2}) \cdot (1+0)} KII e^{1 \cdot \Phi II_j (1-\alpha2)}}$$

$\Phi_{j,r} = \Phi I_{j,r} + \Phi II_{j,r}$

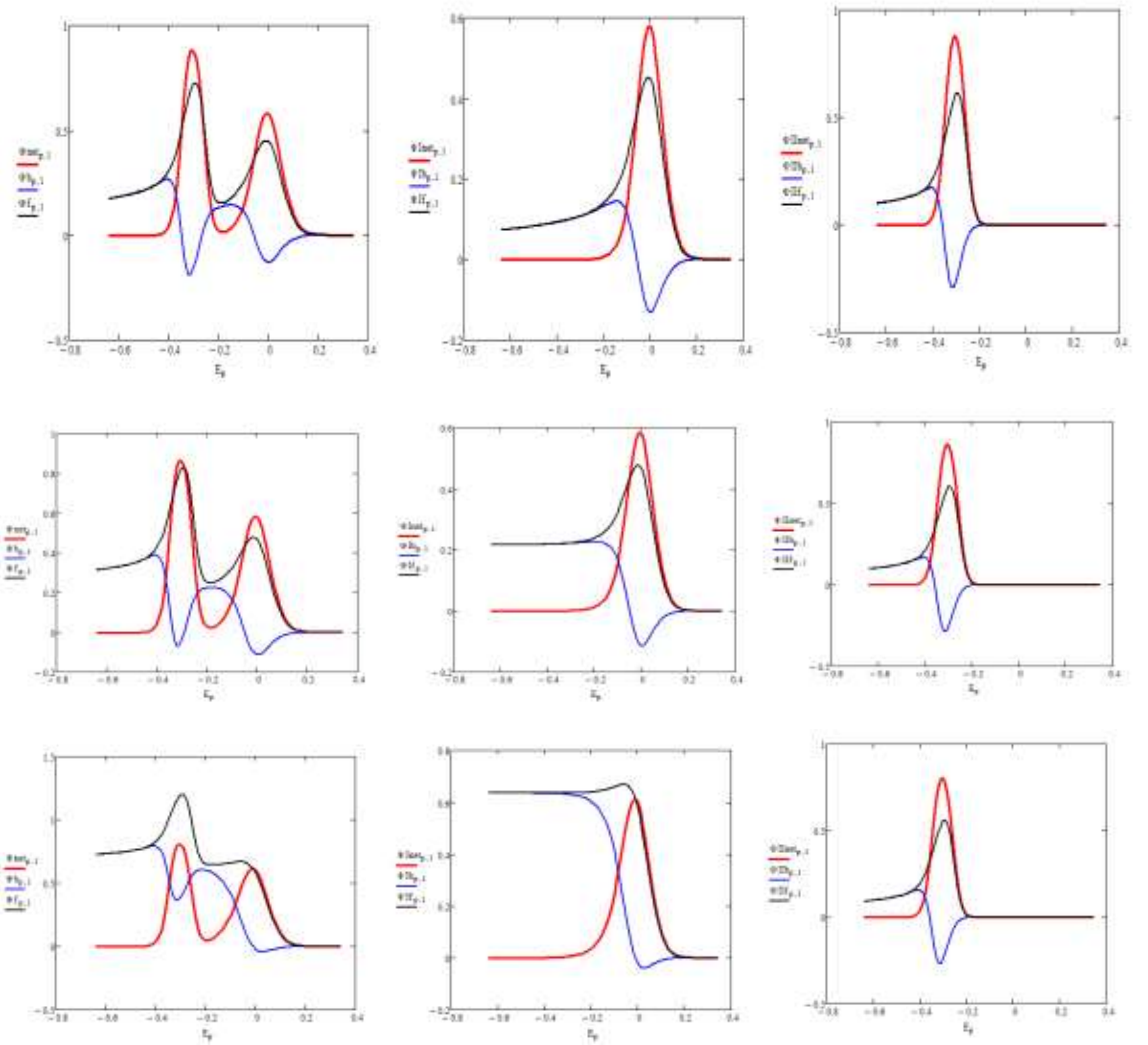
$p = 1 .. \left(\frac{\Delta E}{dE}\right) - 1$

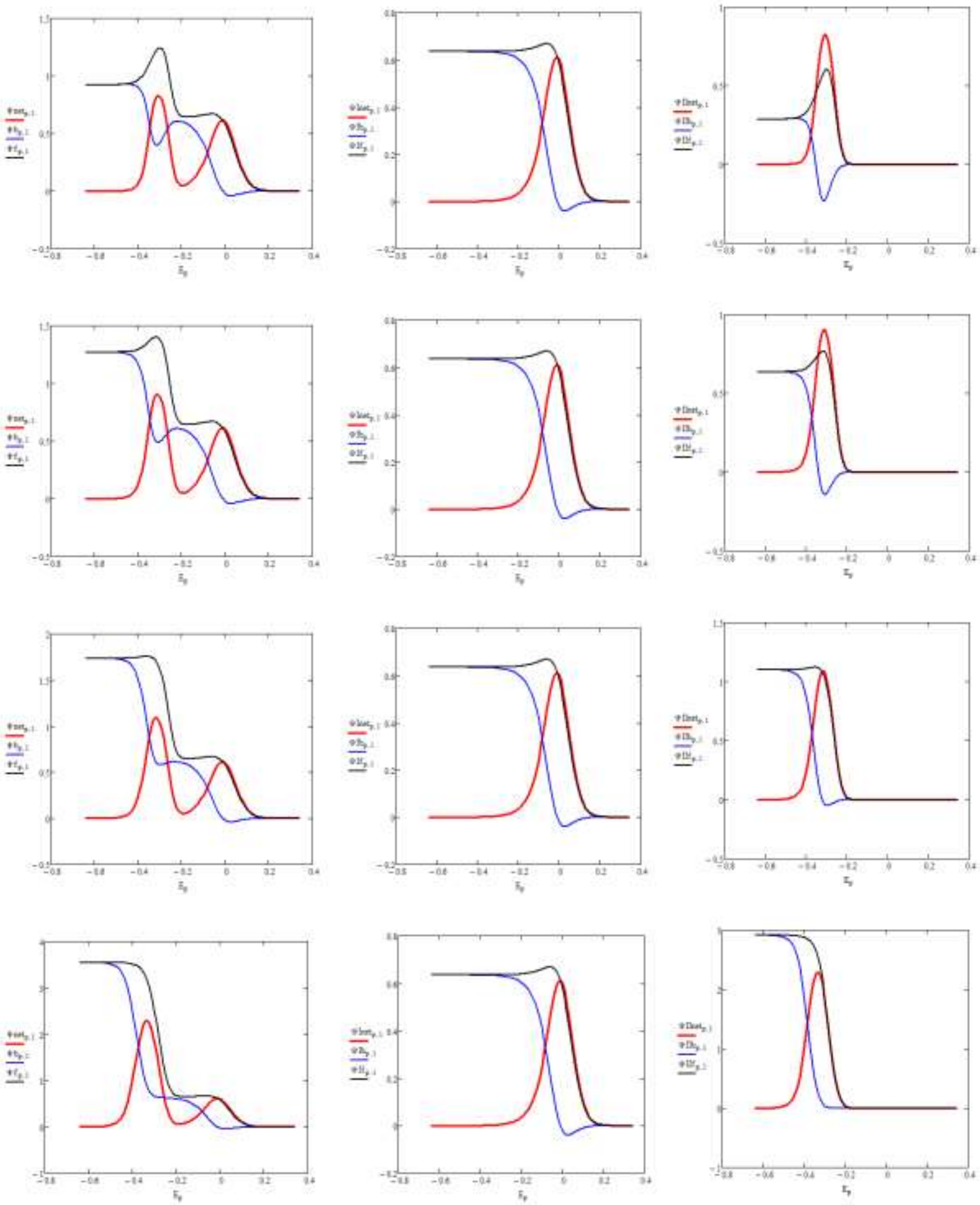
$\Phi If_{p,r} = \Phi I_{(p+1) \cdot 50,r}$ $\Phi Ib_{p,r} = \Phi I_{50 \cdot p+25,r}$ $\Phi Inet_{p,r} = \Phi If_{p,r} - \Phi Ib_{p,r}$

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

$E_p = Esl - p \cdot dE$

$\Phi b_{p,r} = \Phi_{50 \cdot p+25,r}$ $\Phi f_{p,r} = \Phi_{(p+1) \cdot 50,r}$ $\Phi net_{p,r} = \Phi f_{p,r} - \Phi b_{p,r}$





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