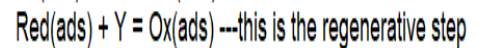
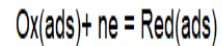


MATHCAD FILE-WORKING SHEET FOR SIMULATION OF SURFACE REGENERATIVE EC' catalytic mechanism (EC'=Electrochemical Mechanism Coupled with Regenerative Chemical Reaction) in SQUARE-WAVE VOLTAMMETRY

Rubin Gulaboski, Valentin Mirceski

$$E_s := 0.25 \quad \Delta E := 0.004 \quad E_{sw} := 0.05$$

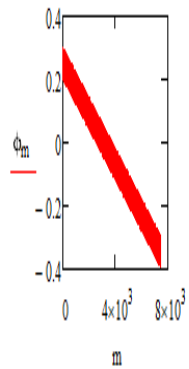


SURFACE CATALYTIC EC' mechanism in Square-wave voltammetry

$$m := 1.. \frac{0.6}{\Delta E} \cdot 50$$

$$\text{relativenpot}_m := \left[\left(\text{ceil} \left(\frac{m}{25} \right) \cdot \Delta E + \text{if} \left(\frac{\text{ceil} \left(\frac{m}{25} \right)}{2} = \text{ceil} \left(\frac{m}{25} \right), 1, -1 \right) \cdot E_{sw} + E_{sw} \right) - \Delta E \right]$$

$$\phi_m := E_s + E_{sw} - \text{relativenpot}_m$$



$$\alpha := 0.5$$

$$F := 96500 \quad n := 2 \quad R := 8.314 \quad T := 273.15 \quad i := 1..1$$

$$\gamma_i := 10^{0.85+i \cdot 0}$$

$$\lambda_i := 10^0$$

$$k := 1.. \frac{0.6}{\Delta E} \cdot 50 \quad M_{k,i} := e^{-\frac{\gamma_i}{50} \cdot (k-1)} - \frac{\gamma_i}{50} \cdot (k)$$

$$\log(\gamma_i) = 0.85$$

$$\gamma_i = 7.0795$$

$$\log(\lambda_i) = 0$$

$$\phi_{em} := \frac{n \cdot F}{R \cdot T} \cdot \phi_m$$

$$I_1 := \lambda_1 \cdot e^{-\alpha \cdot \phi_1} \left[1 + \lambda_1 \cdot e^{-\alpha \cdot \phi_1} \cdot (1 + e^{\phi_1}) \cdot R^{-1} \right]^{-1}$$

$$I_m := \lambda \cdot e^{-\alpha \cdot \phi_m} \left[1 - (1 + e^{\phi_m}) \cdot R^{-1} \cdot \sum_{j=1}^{m-1} I_j \right] \left[1 + \lambda \cdot e^{-\alpha \cdot \phi_m} \cdot (1 + e^{\phi_m}) \cdot R^{-1} \right]^{-1}$$

Povrsinska
reakcija

$$\Psi_{1,i} := \frac{\lambda_1 \cdot e^{-\alpha \cdot \phi_1}}{1 + \lambda_1 \cdot e^{-\alpha \cdot \phi_1} \cdot (1 + e^{\phi_1})} \cdot \frac{M_{1,i}}{\gamma_i}$$

Remark: there is no diffusion in this model

$$I_m := \lambda \cdot e^{-\alpha \cdot \Phi_m} \left[1 - (1 + e^{\Phi_m}) \cdot R^{-1} \cdot \sum_{j=1}^{m-1} I_j \right] \left[1 + \lambda \cdot e^{-\alpha \cdot \Phi_m} (1 + e^{\Phi_m}) \cdot R^{-1} \right]^{-1}$$

$$\Psi_{1,i} := \frac{\lambda_1 \cdot e^{-\alpha \cdot \Phi_1}}{1 + \lambda_1 \cdot e^{-\alpha \cdot \Phi_1} (1 + e^{\Phi_1})} \cdot \frac{M_{1,i}}{\gamma_i}$$

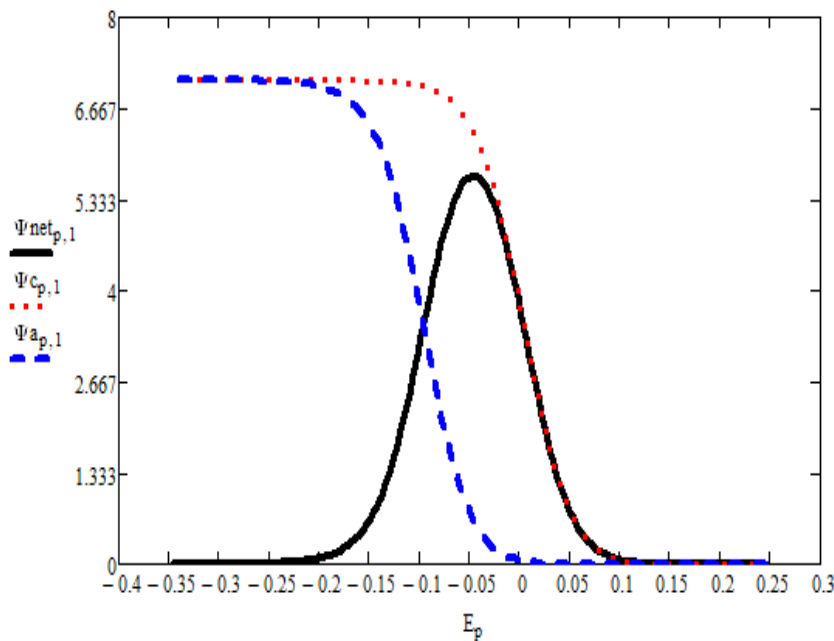
$$\Psi_{m,i} := \frac{\lambda_1 \cdot e^{-\alpha \cdot \Phi_m} \left[1 - \frac{1 + e^{\Phi_m}}{\gamma_i} \cdot \sum_{j=1}^{m-1} [\Psi_{j,i} \cdot M_{(m-j)+1,i}] \right]}{1 + \lambda_1 \cdot e^{-\alpha \cdot \Phi_m} (1 + e^{\Phi_m})} \cdot \frac{M_{1,i}}{\gamma_i}$$

Kataliticka površinska reakcija

$$p := 1 - \frac{0.6}{\Delta E} - 1E_p := E_s - p \cdot \Delta E$$

$$I_{a_p} := I_{50-p+25} \quad I_{c_p} := I_{(p+1) \cdot 50} \quad I_{net_p} := I_{c_p} - I_{a_p}$$

$$\Psi_{a_{p,i}} := \Psi_{50-p+25,i} \quad \Psi_{c_{p,i}} := \Psi_{(p+1) \cdot 50,i} \quad \Psi_{net_{p,i}} := \Psi_{c_{p,i}} - \Psi_{a_{p,i}}$$



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