MATHCAD FILE FOR SIMULATION OF SURFACE CATALYTIC REGENERATIVE MECHANISM IN

CYCLIC VOLTAMMETRY (with IREEVERSIBLE CHEMICAL STEP)

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$tac := 0.01$

$Es := -0.6 \quad Ef := 0.6 \quad \Delta E := Ef - Es \quad dE := 0.01 \quad \tau := 0.01 \quad d := \frac{\tau}{25} \quad s := 1 .. \frac{tac}{d}$

$m := \frac{tac}{d} + 1 .. \frac{\Delta E}{dE} \cdot 25 + \frac{tac}{d} \qquad n := \frac{\Delta E}{dE} \cdot 25 + \frac{tac}{d} + 1 .. \left(\frac{\Delta E}{dE} \cdot 25 \cdot 2 + \frac{tac}{d} \right) \qquad \frac{\Delta E}{dE} = 120$

$el := 2 \qquad \alpha := 0.5$

$E_m := Es + \left(\mathrm{ceil}\left(\frac{m - \frac{tac}{d}}{25} \right) \cdot dE - dE \right)$

$F := 96500 \qquad U := 8.314 \quad T := 298.15$

$\frac{25}{0.04} = 625 \qquad \frac{dE}{\tau} = 1$

$\lambda := .32 \qquad \gamma := 00.000000092$

$E_n := Ef - \left[\mathrm{ceil}\left[\frac{n - \left(\frac{\Delta E}{dE} \cdot 25 + \frac{tac}{d} \right)}{25} \right] \cdot dE - dE \right]$

$k := 1 .. 2 \left(\frac{\Delta E}{dE} \cdot 25 + \frac{tac}{d} \right)$

$M_k := e^{-\frac{\gamma}{25} \cdot (k-1)} - e^{-\frac{\gamma}{25} \cdot (k)}$

SURFACE CATALYTIC MECHANISM EC' in CYCLIC VOLTAMMETRY

- λ is dimensionless kinetic parameter related to electrode reaction
- γ is dimensionless catalytic parameter related to regenerative reactions
- α is electron transfer coefficient
- Es is starting potential
- Ef is final potential
- dE is potential step
- Ψ is symbol for dimensionless current
- Em is cathodic potential ramp in cyclic voltammetry
- En is anodic potential ramp
- Mk is integration factor

$\Phi_m := \frac{el \cdot F}{U \cdot T} \cdot E_m \qquad \Phi_n := \frac{el \cdot F}{U \cdot T} \cdot E_n \qquad \Phi ac := \frac{el \cdot F}{U \cdot T} \cdot Es$

$$\Psi_1 := \frac{\lambda \cdot e^{-\alpha \cdot \Phi_1}}{1 + \lambda \cdot e^{-\alpha \cdot \Phi_1} \cdot \left(1 + e^{\Phi_1}\right) \cdot \frac{M_1}{\gamma}}$$

$$\Psi_s := \frac{\lambda \cdot e^{-\alpha \cdot \Phi ac} \cdot \left[1 - \frac{1 + e^{\Phi ac}}{\gamma} \cdot \sum_{j=1}^{s-1} \left(\Psi_j \cdot M_{s-j+1} \right) \right]}{1 + \lambda \cdot e^{-\alpha \cdot \Phi ac} \cdot \left(1 + e^{\Phi ac}\right) \cdot \frac{M_1}{\gamma}}$$

$$\Psi_m := \frac{\lambda \cdot e^{-\alpha \cdot \Phi_m} \cdot \left[1 - \frac{1 + e^{\Phi_m}}{\gamma} \cdot \sum_{j=1}^{m-1} \left(\Psi_j \cdot M_{m-j+1} \right) \right]}{1 + \lambda \cdot e^{-\alpha \cdot \Phi_m} \cdot \left(1 + e^{\Phi_m}\right) \cdot \frac{M_1}{\gamma}}$$

Katalitcka povrsinska reakcija

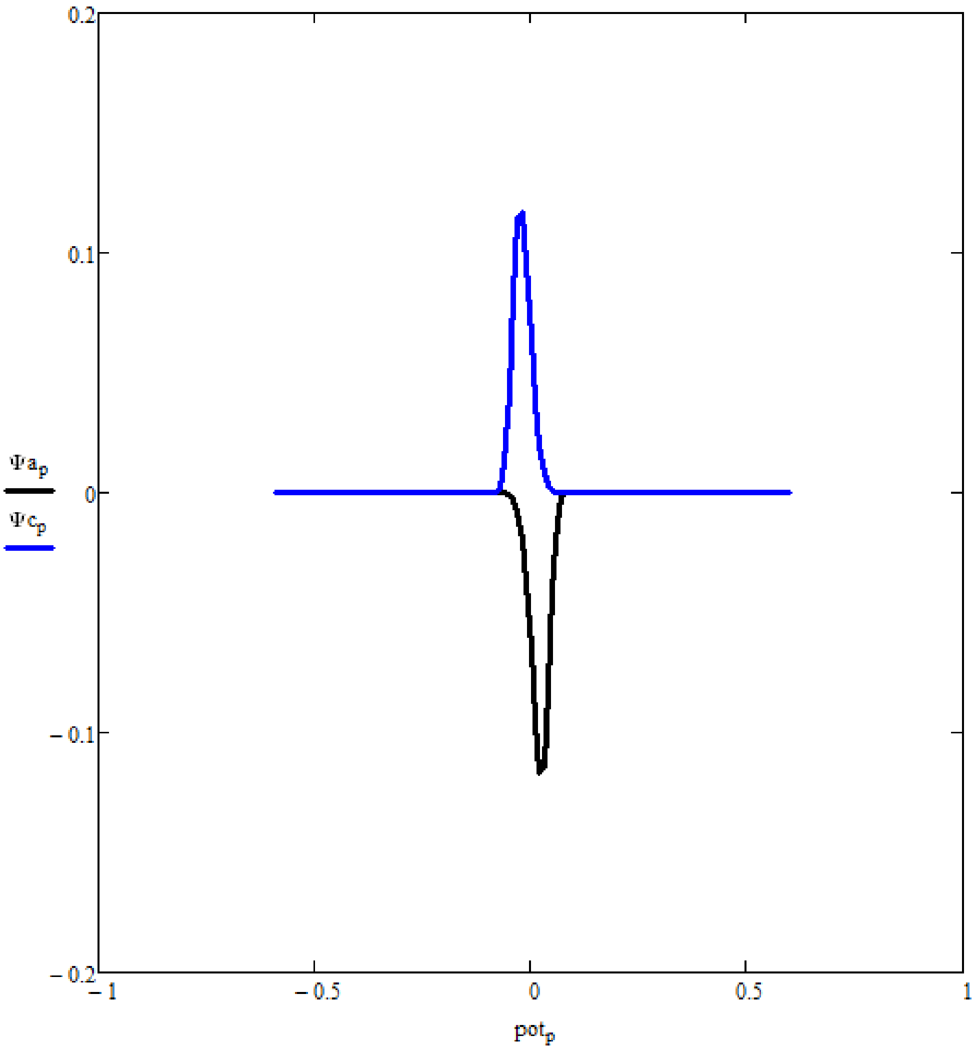
$$\Psi_n := \frac{\lambda \cdot e^{-\alpha \cdot \Phi_n} \cdot \left[1 - \frac{1 + e^{\Phi_n}}{\gamma} \cdot \sum_{j=1}^{n-1} \left(\Psi_j \cdot M_{n-j+1} \right) \right]}{1 + \lambda \cdot e^{-\alpha \cdot \Phi_n} \cdot \left(1 + e^{\Phi_n}\right) \cdot \frac{M_1}{\gamma}}$$

$$p := 1 .. \frac{\Delta E}{dE}$$

$$\Psi a_p := (\Psi)_{\left(\frac{\tau}{d \cdot 25}+p\right) \cdot 25}$$

$$\Psi c_p := (\Psi)_{\left[\left[\frac{\Delta E}{dE} \cdot 2+\left(\frac{\tau}{25 \cdot d}\right)\right]-p\right] \cdot 25}$$

$$pot_p := Es + p \cdot dE$$



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