

MATHCAD FILE FOR SIMULATION OF CATHODIC STRIPPING REACTION OF FIRST ORDER, ASSOCIATED WITH ADSORPTION OF THE LIGAND-CALCULATION FILE IN CYCLIC VOLTAMMETRY

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Abstract

Cathodic Stripping mechanism of first order that is coupled with the adsorption of reacting ligand is simulated under conditions of cyclic staircase voltammetry. The simulation file contains all parameters for calculating cyclic voltammograms of this complex mechanism under conditions of cyclic staircase voltammetry. Model is suitable to study the features of quasireversible electrode systems of many metal-ligand complexes and metal-drug complexes, in which the ligand gets adsorbed at the working electrode surface.

katodna stripping reakcija od I red so adsorpcija na reaktant
Ciklicna skalesta voltmetrija

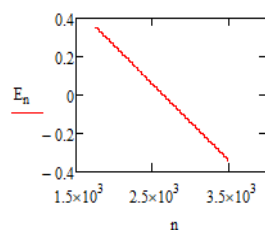
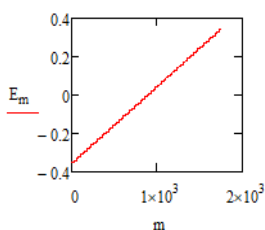
CATHODIC STRIPPING MECHANISM WITH ADSORPTION OF THE LIGAND
REACTION OF FIRST ORDER
SIMULATION IN CYCLIC STAIRCASE VOLTAMMETRY

$$E_s := -0.35 \quad E_f := 0.35 \quad \Delta E := E_f - E_s \quad dE := 0.01 \quad tac := 0.01 \quad \tau := 0.05 \quad d := \frac{\tau}{25}$$

$$s := 1 - \frac{tac}{d} \quad m := \frac{tac}{d} + 1 - \frac{\Delta E}{dE} \cdot 25 + \frac{tac}{d} \quad n := \frac{\Delta E}{dE} \cdot 25 + \frac{tac}{d} + 1 - \left(\frac{\Delta E}{dE} \cdot 25 \cdot 2 + \frac{tac}{d} \right)$$

$$E_m := E_s + \left(\text{ceil} \left(\frac{m - \frac{tac}{d}}{25} \right) \cdot dE - dE \right) \quad \frac{tac}{d} = 5$$

$$E_n := E_f - \left[\text{ceil} \left[\frac{n - \left(\frac{\Delta E}{dE} \cdot 25 + \frac{tac}{d} \right)}{25} \right] \cdot dE - dE \right] \quad \frac{25}{0.04} = 625 \quad \frac{dE}{\tau} = 0.2$$



$$F := 96500 \quad e1 := 2 \quad R := 8.314 \quad T := 298.15 \quad Ks := 1 \quad Kads := 1$$

$$D := 5 \cdot 10^{-6} \quad a := \sqrt{D} \cdot Kads \quad \phi_{m} := e1 \cdot \frac{F}{R \cdot T} \cdot (E_m) \quad \phi_n := e1 \cdot \frac{F}{R \cdot T} \cdot (E_n) \quad \rho := a \cdot \sqrt{2} \cdot \tau \quad \rho = 7.071 \times 10^{-4}$$

$$\Phi_{ac} := eI \cdot \frac{F}{R \cdot T} \cdot Es \quad \alpha := 0.5 \quad \lambda := \frac{Ks \cdot \sqrt{2 \cdot \tau}}{\sqrt{D}} \quad \gamma := \sqrt{D \cdot 2 \cdot \tau} \quad k := 1.2 \cdot \left(\frac{\Delta E}{dE} \cdot 25 + \frac{tac}{d} \right) \quad \omega := \lambda \cdot \gamma$$

$$R_{\omega k} := e^{\left[\frac{(a)^2}{k} \right] \cdot k \cdot d} \cdot (1 - \operatorname{erf}(a \cdot \sqrt{k \cdot d})) - e^{\left[\frac{(a)^2}{(k-1)} \right] \cdot (k-1) \cdot d} \cdot [1 - \operatorname{erf}[\sqrt{(k-1) \cdot d} \cdot a]] \quad S_{\omega k} := \sqrt{k} - \sqrt{k-1}$$

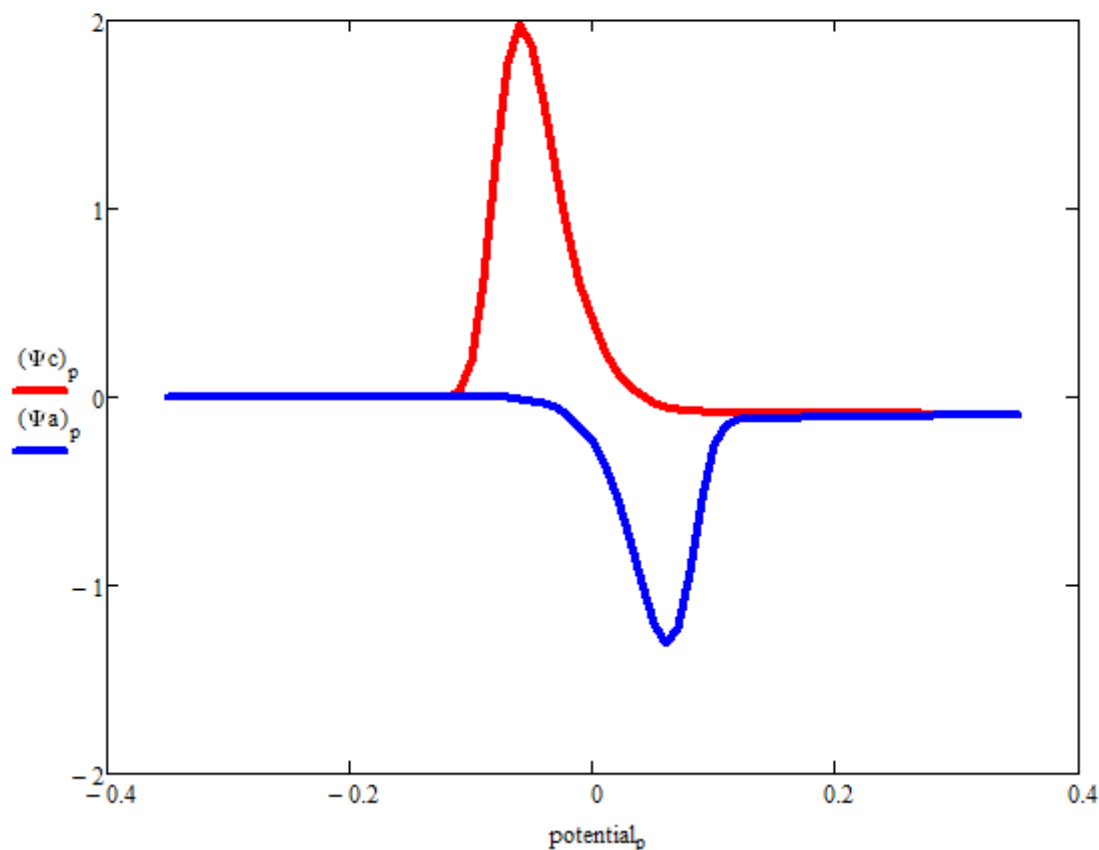
$$\Psi_1 := \frac{-\lambda \cdot e^{(1-\alpha) \cdot \Phi_{ac}} \left[1 - e^{\left[\frac{(\rho)^2 \cdot 1}{50} \right]} \cdot \left(1 - \operatorname{erf} \left(\rho \cdot \sqrt{\frac{1}{50}} \right) \right) \right]}{1 + \frac{\lambda \cdot \gamma}{50} \cdot e^{-\alpha \cdot \Phi_{ac}} + \frac{\lambda \cdot e^{(1-\alpha) \cdot \Phi_{ac}} \cdot \left(\frac{2 \cdot S_1}{\sqrt{\pi}} + \frac{\sqrt{50} \cdot R_1}{\rho} \right)}{\sqrt{50}}}$$

$$\Psi_s := \frac{\frac{-\lambda \cdot \gamma \cdot e^{-\alpha \cdot \Phi_{ac}}}{50} \cdot \sum_{i=1}^{s-1} \Psi_i - \lambda \cdot e^{(1-\alpha) \cdot \Phi_{ac}} \left[1 - e^{\left[\frac{(\rho)^2 \cdot s}{50} \right]} \cdot \left(1 - \operatorname{erf} \left(\rho \cdot \sqrt{\frac{s}{50}} \right) \right) \right] + \frac{1}{\sqrt{50}} \cdot \sum_{i=1}^{s-1} \left[\Psi_i \cdot \left[\frac{2 \cdot S_{s-i+1}}{\sqrt{\pi}} + \frac{\sqrt{50} \cdot R_{(s-i)+1}}{\rho} \right] \right]}{1 + \frac{\lambda \cdot \gamma}{50} \cdot e^{-\alpha \cdot \Phi_{ac}} + \frac{\lambda \cdot e^{(1-\alpha) \cdot \Phi_{ac}} \cdot \left(\frac{2 \cdot S_1}{\sqrt{\pi}} + \frac{\sqrt{50} \cdot R_1}{\rho} \right)}{\sqrt{50}}}$$

$$\Psi_m := \frac{\frac{-\lambda \cdot \gamma \cdot e^{-\alpha \cdot \Phi_m}}{50} \cdot \sum_{i=1}^{m-1} \Psi_i - \lambda \cdot e^{(1-\alpha) \cdot \Phi_m} \left[1 - e^{\left[\frac{(\rho)^2 \cdot m}{50} \right]} \cdot \left(1 - \operatorname{erf} \left(\rho \cdot \sqrt{\frac{m}{50}} \right) \right) \right] + \frac{1}{\sqrt{50}} \cdot \sum_{i=1}^{m-1} \left[\Psi_i \cdot \left[\frac{2 \cdot S_{m-i+1}}{\sqrt{\pi}} + \frac{\sqrt{50} \cdot R_{(m-i)+1}}{\rho} \right] \right]}{1 + \frac{\lambda \cdot \gamma}{50} \cdot e^{-\alpha \cdot \Phi_m} + \frac{\lambda \cdot e^{(1-\alpha) \cdot \Phi_m} \cdot \left(\frac{2 \cdot S_1}{\sqrt{\pi}} + \frac{\sqrt{50} \cdot R_1}{\rho} \right)}{\sqrt{50}}}$$

$$\Psi_n := \frac{\frac{-\lambda \cdot \gamma \cdot e^{-\alpha \cdot \Phi_n}}{50} \cdot \sum_{i=1}^{n-1} \Psi_i - \lambda \cdot e^{(1-\alpha) \cdot \Phi_n} \left[1 - e^{\left[\frac{(\rho)^2 \cdot n}{50} \right]} \cdot \left(1 - \operatorname{erf} \left(\rho \cdot \sqrt{\frac{n}{50}} \right) \right) \right] + \frac{1}{\sqrt{50}} \cdot \sum_{i=1}^{n-1} \left[\Psi_i \cdot \left[\frac{2 \cdot S_{n-i+1}}{\sqrt{\pi}} + \frac{\sqrt{50} \cdot R_{(n-i)+1}}{\rho} \right] \right]}{1 + \frac{\lambda \cdot \gamma}{50} \cdot e^{-\alpha \cdot \Phi_n} + \frac{\lambda \cdot e^{(1-\alpha) \cdot \Phi_n} \cdot \left(\frac{2 \cdot S_1}{\sqrt{\pi}} + \frac{\sqrt{50} \cdot R_1}{\rho} \right)}{\sqrt{50}}}$$

$$p := 0.. \frac{\Delta E}{dE} \quad \Psi_{a_p} := \Psi \left(\frac{tac}{d \cdot 25} + p \right) \cdot 25 \quad \Psi_{c_p} := \Psi \left[\left[\frac{\Delta E}{dE} \cdot 2 + \left(\frac{tac}{25 \cdot d} \right) \right] - p \right] \cdot 25 \quad \text{potential}_{(p)} := E_s + p \cdot dE$$



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