Electrochemically Induced Irreversible Dimerization in Cyclic Voltammetry- MATHCAD Simulation Protocol

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$tac := 0.01$

$Es := -0.4$ $Ef := 0.4$ $\Delta E := Ef - Es$ $dE := 0.004$ $\tau := 0.01$ $d := \frac{\tau}{25}$ $cs := .000075$

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

$\frac{\Delta E}{dE} = 200$

$el := 1$ $\alpha := 0.5$ $E_m := Es + \left(ceil\left(\frac{m - \frac{\tau}{d}}{25}\right) \cdot dE - dE\right)$ $E_n := Ef - \left[ceil\left[\frac{n - \left(\frac{\Delta E}{dE} \cdot 25 + \frac{\tau}{d}\right)}{25}\right] \cdot dE - dE\right]$

$F := 96500$ $R := 8.314$ $T := 298.15$

$Keq := 10.00$

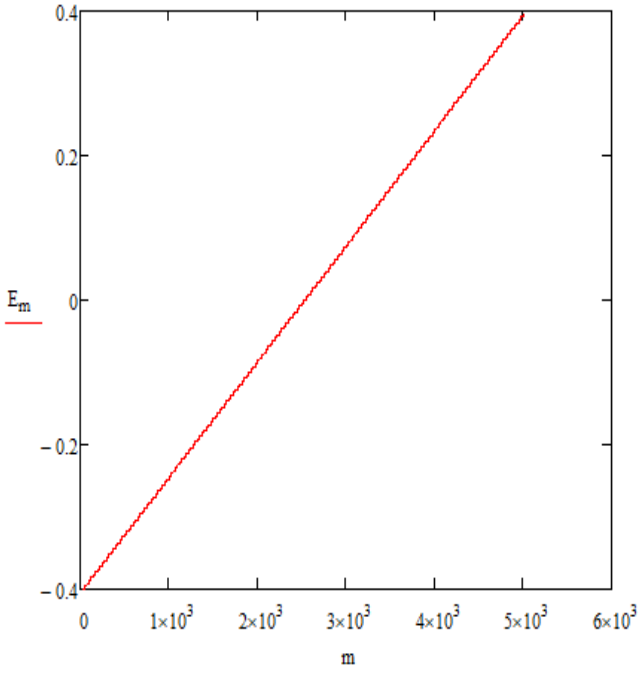
$k := 1 .. 2 \cdot \left(\frac{\Delta E}{dE} \cdot 25 + \frac{\tau}{d}\right)$ $ks := 1.0$

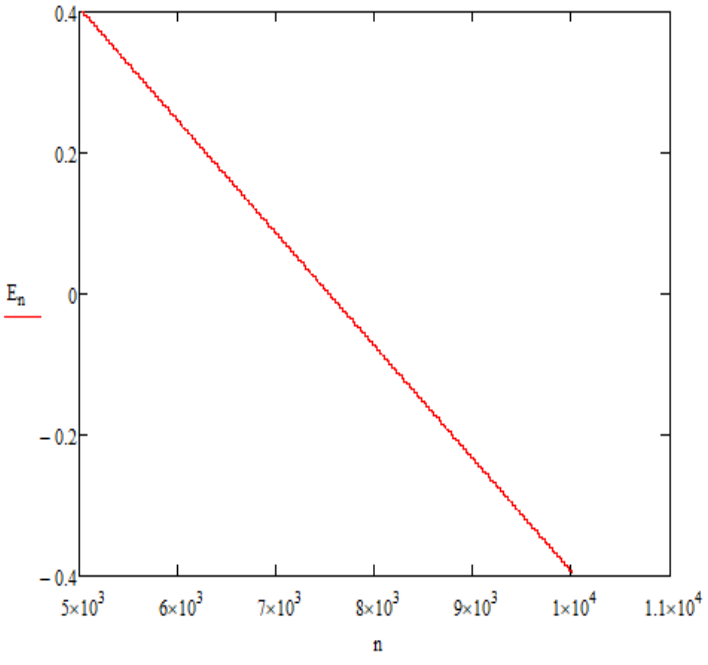
$\varepsilon := .001$

$\Phi_m := \frac{el \cdot F}{R \cdot T} \cdot E_m$ $\Phi_n := \frac{el \cdot F}{R \cdot T} \cdot E_n$ $\Phi ac := \frac{el \cdot F}{R \cdot T} \cdot Es$ $K := ks \cdot \tau$

$K = 0.01$ $Kchem := \frac{\varepsilon \cdot \tau}{1}$ $Kchem = 1 \times 10^{-5}$

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



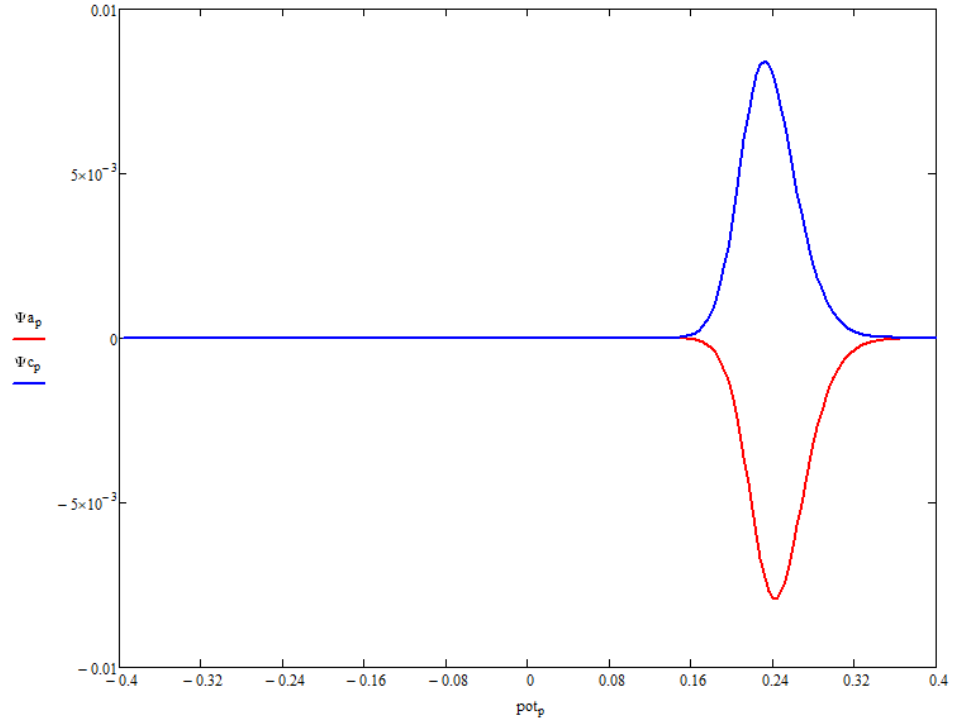


$$\Psi_s := \frac{\frac{K}{cs}\cdot e^{-\alpha\cdot\Phi ac}}{1+\frac{K}{25\cdot cs}\cdot e^{-\alpha\cdot\Phi ac}+\frac{1}{1^1}\cdot\left[1K\,Kchem^{-1}\cdot e^{\Phi ac\cdot(1-\alpha)}\cdot M_1\right]^2}$$

$$\Psi_m := \frac{\frac{K}{cs}\cdot e^{-\alpha\cdot\Phi_m}-\frac{K}{25\cdot cs}\cdot e^{-\alpha\cdot\Phi_m}\cdot\sum_{j=1}^{m-1}\Psi_j-\left(\frac{1}{1^1}\right)\cdot\left[1K\,Kchem^{-1}\cdot e^{\Phi_m\cdot(1-\alpha)}\cdot\sum_{j=1}^{m-1}\left(\Psi_j\cdot M_{m-j+1}\right)\right]^2}{1+\frac{K}{25\cdot cs}\cdot e^{-\alpha\cdot\Phi_m}+\frac{1}{1^1}\cdot\left[1K\,Kchem^{-1}\cdot e^{\Phi_m\cdot(1-\alpha)}\cdot M_1\right]^2}$$

$$+1\Big) \qquad \Psi_n := \frac{\frac{K}{cs}\cdot e^{-\alpha\cdot\Phi_n}-\frac{K}{25\cdot cs}\cdot e^{-\alpha\cdot\Phi_n}\cdot\sum_{j=1}^{n-1}\Psi_j-\left(\frac{1}{1^1}\right)\cdot\left[1K\,Kchem^{-1}\cdot e^{\Phi_n\cdot(1-\alpha)}\cdot\sum_{j=1}^{n-1}\left(\Psi_j\cdot M_{n-j+1}\right)\right]^2}{1+\frac{K}{25\cdot cs}\cdot e^{-\alpha\cdot\Phi_n}+\frac{1}{1^1}\cdot\left[1K\,Kchem^{-1}\cdot e^{\Phi_n\cdot(1-\alpha)}\cdot M_1\right]^2}$$

$pot_p := Es + p\cdot dE$



C = 0.000075

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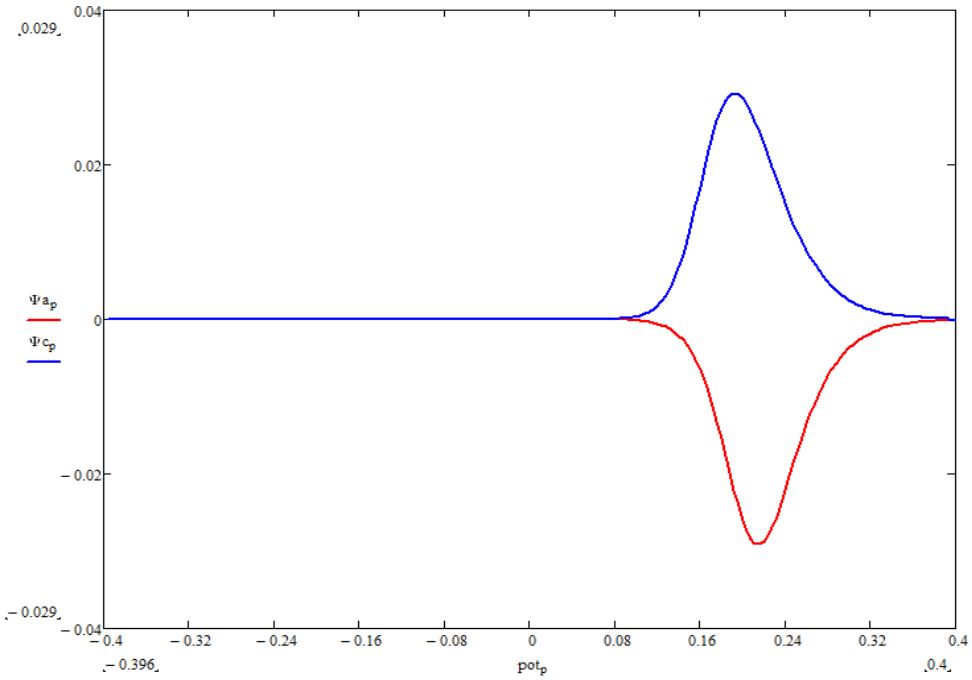
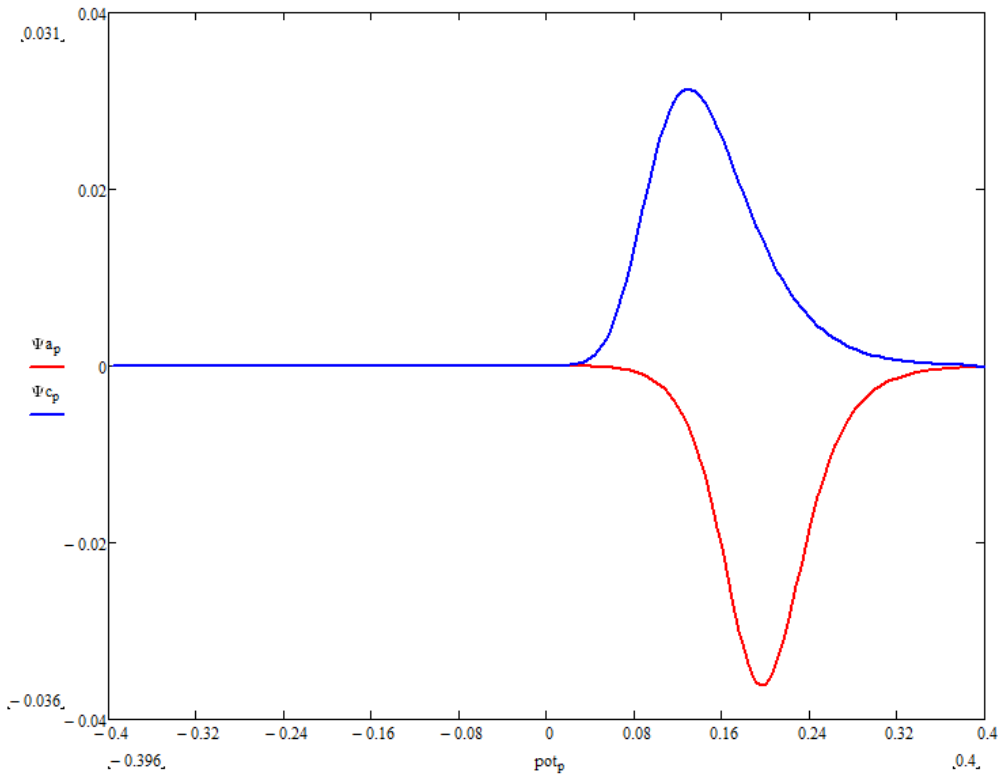


C = 0.0075



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