# MATHCAD platform for calculating cyclic voltammograms


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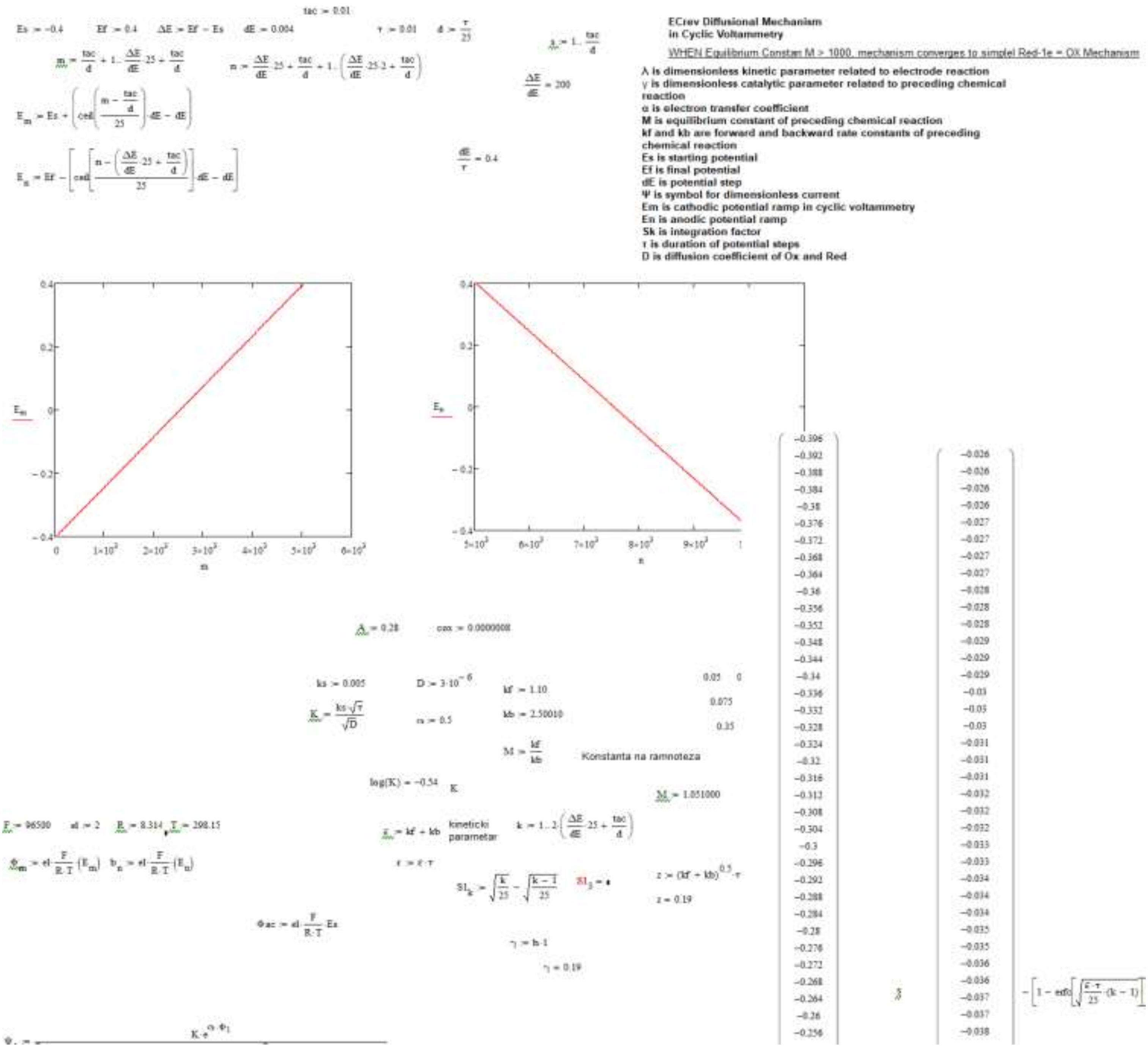
**Abstract:**

A practical on-line MATHCAD simulation platform, which can be used to calculate cyclic voltammograms of simple Red -1e- = Ox mechanism, is presented. The platform is free to use for everyone. In a series of such simulation platforms, we gonna provide all MATHCAD files needed to calculate cyclic voltammograms of all relevant electrochemical mechanisms.

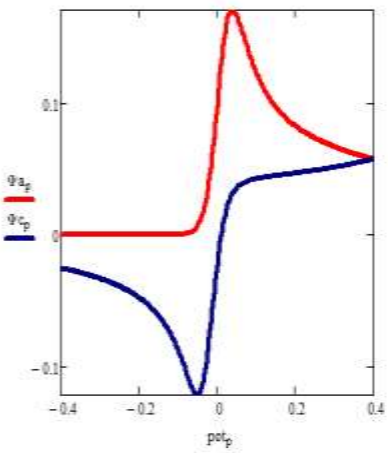
$$\Psi_1 := \frac{K \cdot e^{\alpha \cdot \Phi_1}}{\left[1 + \frac{1 \cdot K \cdot e^{-(1-\alpha)\cdot \Phi_1}}{\sqrt{\pi \cdot 1}} + \frac{1 \cdot K \cdot e^{-(1-\alpha)\cdot \Phi_1}}{\sqrt{\pi \cdot 1}} \cdot \frac{M}{1+M}\right] + \frac{\gamma}{1+M} \cdot e^{-(1-\alpha)\cdot \Phi_1} \cdot S_1}$$

$$\Psi_s := \frac{K \cdot e^{\alpha \cdot \Phi ac} - \frac{2 \cdot K \cdot e^{\alpha \cdot \Phi ac}}{\sqrt{\pi \cdot 1}} \cdot \sum_{j=1}^{s-1} \left(\Psi_j \cdot S1_{s-j+1}\right) - \frac{2 \cdot K \cdot e^{-(1-\alpha)\cdot \Phi ac}}{\sqrt{\pi \cdot 1}} \cdot \frac{M}{1+M} \cdot \sum_{j=1}^{s-1} \left(\Psi_j \cdot S1_{s-j+1}\right) - \frac{\gamma}{1+M} \cdot e^{-(1-\alpha)\cdot \Phi ac} \cdot \sum_{j=1}^{s-1} \left(\Psi_j \cdot S_{s-j+1}\right)}{1 + \frac{2 \cdot K \cdot e^{\alpha \cdot \Phi ac}}{\sqrt{\pi \cdot 1}} + \frac{2 \cdot K \cdot e^{-(1-\alpha)\cdot \Phi ac}}{\sqrt{\pi \cdot 1}} \cdot \frac{M}{1+M} + \frac{\gamma}{1+M} \cdot e^{-(1-\alpha)\cdot \Phi ac} \cdot S_1}$$

$$\Psi_m := \frac{K \cdot e^{\alpha \cdot \Phi_m} - \frac{2 \cdot K \cdot e^{\alpha \cdot \Phi_m}}{\sqrt{\pi \cdot 1}} \cdot \sum_{j=1}^{m-1} \left(\Psi_j \cdot S1_{m-j+1}\right) - \frac{2 \cdot K \cdot e^{-(1-\alpha)\cdot \Phi_m}}{\sqrt{\pi \cdot 1}} \cdot \frac{M}{1+M} \cdot \sum_{j=1}^{m-1} \left(\Psi_j \cdot S1_{m-j+1}\right) - \frac{\gamma}{1+M} \cdot e^{-(1-\alpha)\cdot \Phi_m} \cdot \sum_{j=1}^{m-1} \left(\Psi_j \cdot S_{m-j+1}\right)}{1 + \frac{2 \cdot K \cdot e^{\alpha \cdot \Phi_m}}{\sqrt{\pi \cdot 1}} + \frac{2 \cdot K \cdot e^{-(1-\alpha)\cdot \Phi_m}}{\sqrt{\pi \cdot 1}} \cdot \frac{M}{1+M} + \frac{\gamma}{1+M} \cdot e^{-(1-\alpha)\cdot \Phi_m} \cdot S_1}$$

$$\Psi_n := \frac{K \cdot e^{\alpha \cdot b_n} - \frac{2 \cdot K \cdot e^{\alpha \cdot b_n}}{\sqrt{\pi \cdot 1}} \cdot \sum_{j=1}^{n-1} \left(\Psi_j \cdot S1_{n-j+1}\right) - \frac{2 \cdot K \cdot e^{-(1-\alpha)\cdot b_n}}{\sqrt{\pi \cdot 1}} \cdot \frac{M}{1+M} \cdot \sum_{j=1}^{n-1} \left(\Psi_j \cdot S1_{n-j+1}\right) - \frac{\gamma}{1+M} \cdot e^{-(1-\alpha)\cdot b_n} \cdot \sum_{j=1}^{n-1} \left(\Psi_j \cdot S_{n-j+1}\right)}{1 + \frac{2 \cdot K \cdot e^{\alpha \cdot b_n}}{\sqrt{\pi \cdot 1}} + \frac{2 \cdot K \cdot e^{-(1-\alpha)\cdot b_n}}{\sqrt{\pi \cdot 1}} \cdot \frac{M}{1+M} + \frac{\gamma}{1+M} \cdot e^{-(1-\alpha)\cdot b_n} \cdot S_1}$$

$p := 1 .. \frac{\Delta E}{dE}$ $\quad \Psi a_p := (\Psi)_{\left(\frac{\tau}{d \cdot 25} + p\right) \cdot 25}$ $\quad \Psi c_p := (\Psi)_{\left[\left[\frac{\Delta E}{dE} \cdot 2 + \left(\frac{\tau}{25 \cdot d}\right)\right] - p\right] \cdot 25}$ $\quad pot_p := Es + p \cdot dE$




| | | |
|---|---|---|
| −0.26 | | −0.037 |
| −0.256 | | −0.038 |
| −0.252 | | −0.038 |
| −0.248 | | −0.039 |
| −0.244 | | −0.039 |
| −0.24 | | −0.04 |
| −0.236 | | −0.04 |
| −0.232 | | −0.041 |
| −0.228 | | −0.042 |
| −0.224 | | −0.042 |
| −0.22 | | −0.043 |
| −0.216 | | −0.044 |
| −0.212 | | −0.044 |
| −0.208 | | −0.045 |
| −0.204 | | −0.046 |
| −0.2 | | −0.047 |
| −0.196 | | −0.047 |
| −0.192 | | −0.048 |
| −0.188 | | −0.049 |
| −0.184 | | −0.05 |
| −0.18 | | −0.051 |
| −0.176 | | −0.052 |
| −0.172 | | −0.053 |
| −0.168 | | −0.054 |
| −0.164 | | −0.055 |
| −0.16 | | −0.056 |
| −0.156 | | −0.058 |
| −0.152 | | −0.059 |
| −0.148 | | −0.06 |
| −0.144 | | −0.062 |
| −0.14 | | −0.063 |
| −0.136 | | −0.065 |
| −0.132 | | −0.066 |
| −0.128 | | −0.068 |
| −0.124 | | −0.07 |
| −0.12 | | −0.072 |
| −0.116 | | −0.074 |
| −0.112 | | −0.076 |
| −0.108 | | −0.079 |
| −0.104 | | −0.081 |
| −0.1 | | −0.084 |
| −0.096 | silon =K/25( | −0.087 |
| −0.092 | | −0.09 |
| −0.088 | | −0.093 |
| −0.084 | | −0.096 |
| −0.08 | $\Psi c_p =$ | −0.1 |
| −0.076 | | −0.103 |
| −0.072 | | −0.107 |
| −0.068 | | −0.11 |
| −0.064 | | −0.113 |
| −0.06 | | −0.116 |
| −0.056 | | −0.119 |

$D_s = 0.000002$

$Ic_p = \Phi c_p \cdot 0.5 \cdot F \cdot A \cdot 0.446 \cdot \sqrt[2]{D} \cdot \frac{c00}{\sqrt[2]{\tau}}$

$Ia_p = \Phi a_p \cdot F \cdot 0.5 \cdot A \cdot 0.446 \cdot \sqrt[2]{D} \cdot \frac{c00}{\sqrt[2]{\tau}}$

$Ra := 10000$

$piot_p = Ex + p \cdot dE - (Ic_p - Ia_p) \cdot Ra$

$\sqrt[2]{-1} \cdot -1 = -i$

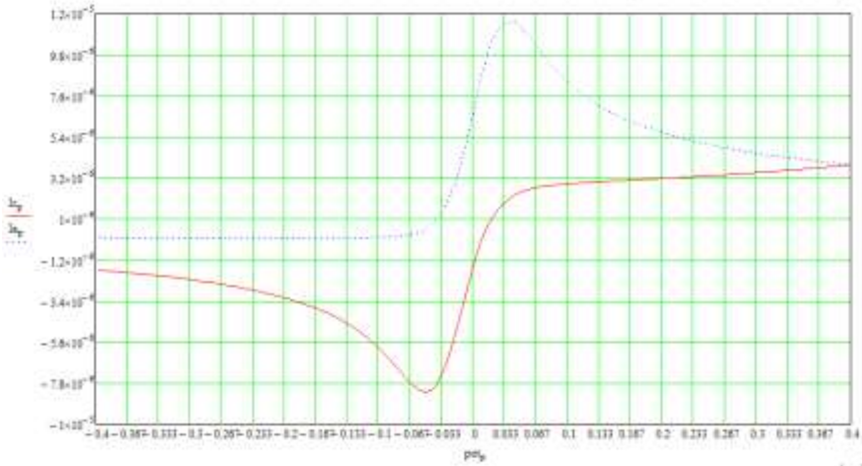
$Ic_{70} = -3.038 \times 10^{-8}$

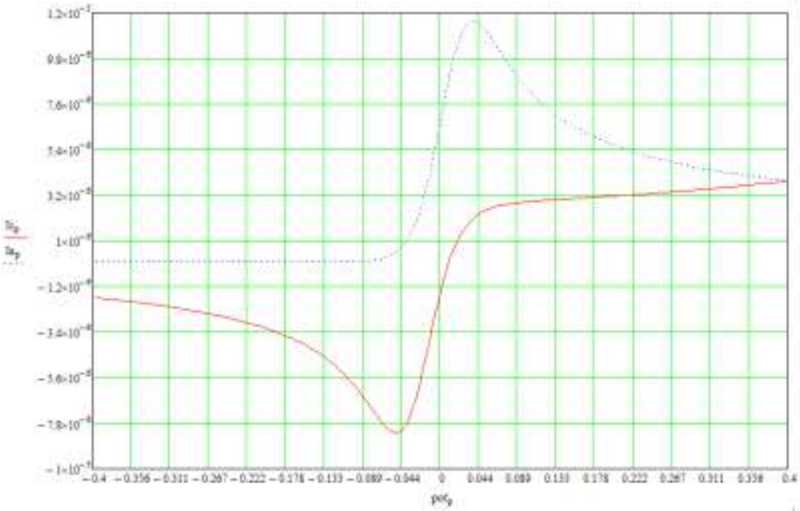
$Ic_{70} \cdot R = -4.285 \times 10^{-7}$

$\frac{1.2}{1.6} = 0.75$

$\frac{1.43}{2.2} = 0.859$

$4.5 \cdot \frac{100}{2.15} = 209.302$




$pot_p =$

| |
|---|
| $-8 \times 10^{-3}$ |
| $-4 \times 10^{-3}$ |
| 0 |
| $4 \times 10^{-3}$ |
| $8 \times 10^{-3}$ |
| 0.012 |
| 0.016 |
| 0.02 |
| 0.024 |
| 0.028 |
| 0.044 |
| 0.048 |
| 0.052 |
| 0.056 |
| 0.06 |
| 0.064 |
| 68 |
| 72 |
| 76 |
| 8 |
| 84 |
| 88 |
| 92 |
| 96 |
| 1 |
| 04 |
| 08 |
| 12 |
| 16 |
| 12 |
| 24 |
| 28 |
| 32 |
| 36 |
| 14 |
| 44 |
| 48 |
| 52 |
| 56 |
| 0.16 |
| 0.164 |
| 0.168 |
| 0.172 |
| 0.176 |
| 0.18 |
| 0.184 |
| 0.188 |
| 0.192 |
| 0.196 |
| 0.2 |
| 0.204 |
| 0.208 |
| 0.212 |
| 0.216 |
| 0.22 |
| 0.224 |
| 0.228 |
| 0.232 |
| 0.236 |
| 0.24 |
| 0.244 |
| 0.248 |
| 0.252 |
| 0.256 |
| 0.26 |
| 0.264 |
| 0.268 |
| 0.272 |
| 0.276 |
| 0.28 |
| 0.284 |
| 0.288 |
| 0.292 |
| 0.296 |

$\Phi c_p =$

| |
|---|
| -0.055 |
| -0.044 |
| -0.033 |
| -0.023 |
| -0.013 |
| $-3.017 \times 10^{-3}$ |
| $2.426 \times 10^{-3}$ |
| $8.882 \times 10^{-3}$ |
| 0.014 |
| 0.019 |
| 0.023 |
| 0.026 |
| 0.029 |
| 0.031 |
| 0.033 |
| 0.035 |
| 0.036 |
| 0.037 |
| 0.038 |
| 0.039 |
| 0.039 |
| 0.04 |
| 0.04 |
| 0.041 |
| 0.041 |
| 0.041 |
| 0.042 |
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| 0.05 |
| 0.05 |
| 0.05 |
| 0.05 |
| 0.051 |
| 0.051 |

$pot_p =$ $Ic_p =$ $Ia_p =$

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