Assessing Activity of Dental Metallic Biomaterials from Cyclic Voltammetry- Effect of the Kinetics of Electron Transfer and the Kinetics of Coupled Chemical Reaction

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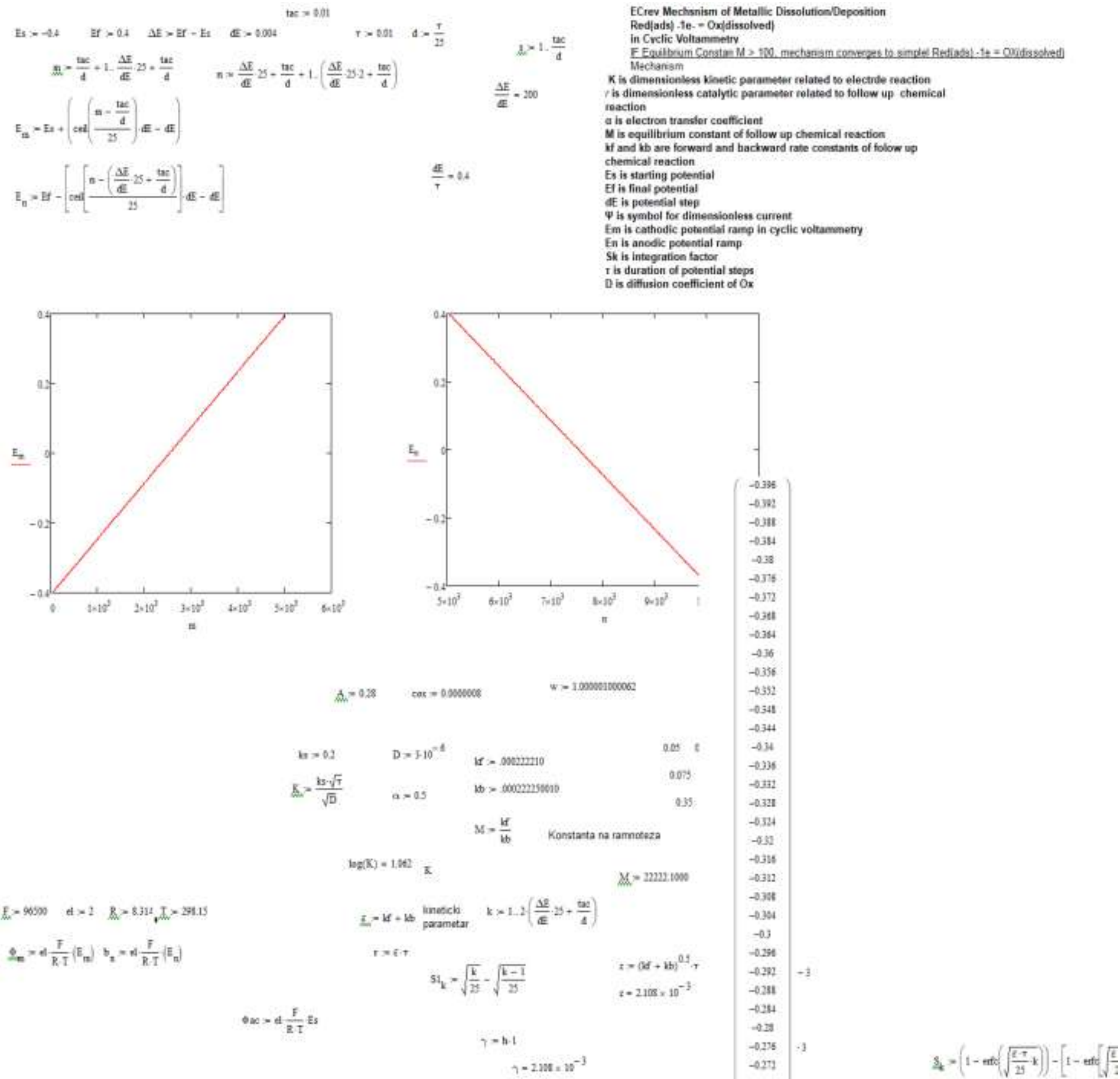
Abstract: In this work, we present set of results obtained from MATHCAD simulation protocol performed in conditions of cyclic voltammetry. Model is related to assess the activity of dental metallic biomaterials in presence of chemical systems that get into interactions with the dental metallic material. The results show how the temperature, the kinetics of electron transfer step, and the kinetics of coupled chemical reaction affect the activity of the metallic dental biomaterial. Results are relevant to study dissolution of metallic biomaterials.



$$\Phi ac := el \cdot \frac{F}{R \cdot T} \cdot Es$$

$$\gamma := h \cdot 1$$

$$\gamma = 2.108 \times 10^{-3}$$

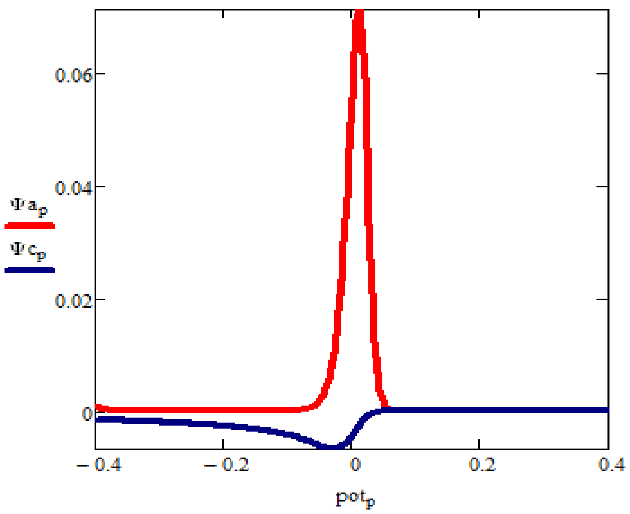
$$\Psi_1 := \frac{K \cdot e^{\alpha \cdot \Phi_1}}{\left[1 + \frac{0.04 \cdot K \cdot e^{(1-\alpha) \cdot \Phi_1} \cdot 1}{\sqrt{1 \cdot 1}} + \frac{1 \cdot K \cdot e^{-(1-\alpha) \cdot \Phi_1}}{\sqrt{\pi \cdot 1}} \cdot \frac{M}{1+M}\right] + \frac{\gamma}{1+M} \cdot e^{-(1-\alpha) \cdot \Phi_1} \cdot S_1}$$

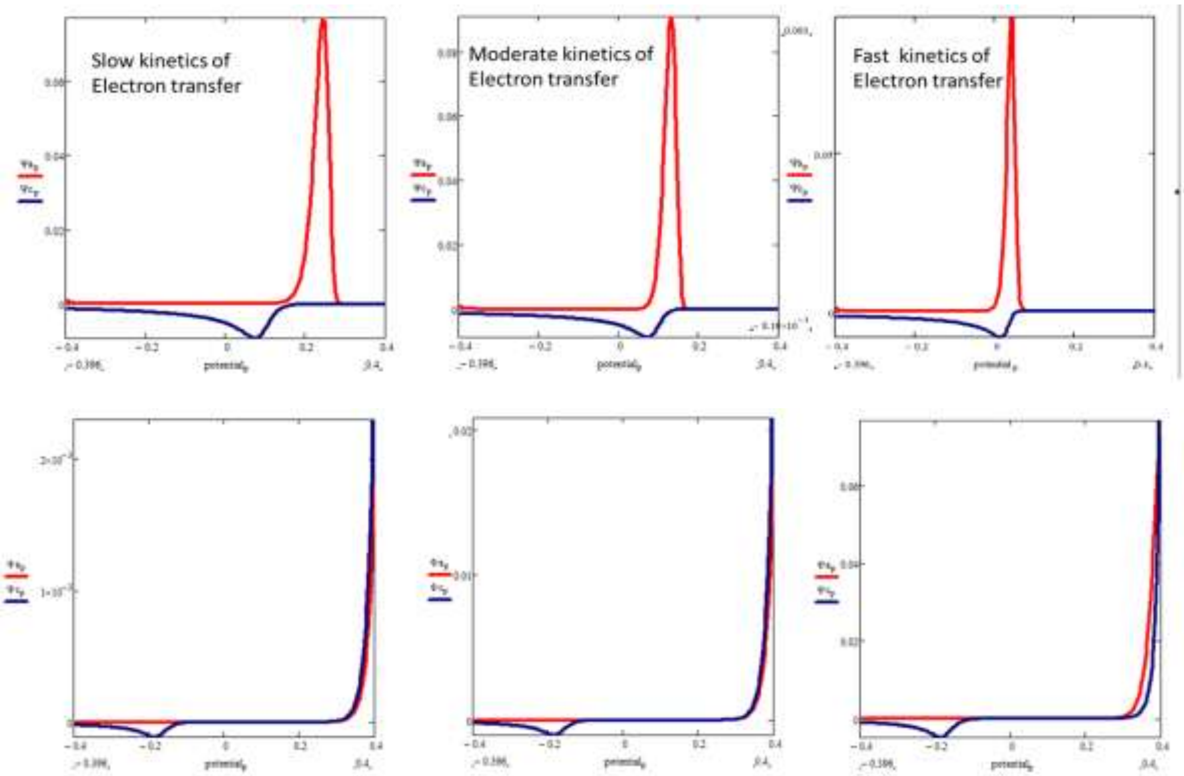
$$\Psi_s := \frac{K \cdot e^{\alpha \cdot \Phi ac} - \frac{0.04 \cdot K \cdot e^{\alpha \cdot \Phi ac}}{\sqrt{1 \cdot 1}} \cdot \sum_{j=1}^{s-1} \left(\Psi_j \cdot 1\right) - \frac{2 \cdot K \cdot e^{-(1-\alpha) \cdot \Phi ac}}{\sqrt{\pi \cdot 25}} \cdot \frac{M}{1+M} \cdot \sum_{j=1}^{s-1} \left(\Psi_j \cdot S1_{s-j+1}\right) - \frac{\gamma}{1+M} \cdot e^{-(1-\alpha) \cdot \Phi ac} \cdot \sum_{j=1}^{s-1} \left(\Psi_j \cdot S_{s-j+1}\right)}{1 + \frac{0.04 \cdot K \cdot e^{\alpha \cdot \Phi ac} \cdot 1}{\sqrt{1 \cdot 1}} + \frac{2 \cdot K \cdot e^{-(1-\alpha) \cdot \Phi ac}}{\sqrt{\pi \cdot 25}} \cdot \frac{M}{1+M} + \frac{\gamma}{1+M} \cdot e^{-(1-\alpha) \cdot \Phi ac} \cdot S_1}$$

$$\Psi_m := \frac{w \cdot e^{\alpha \cdot \Phi_m} - \frac{0.04 \cdot w \cdot e^{\alpha \cdot \Phi_m}}{\sqrt{1 \cdot 1}} \cdot \sum_{j=1}^{m-1} \left(\Psi_j \cdot 1\right) - \frac{2 \cdot K \cdot e^{-(1-\alpha) \cdot \Phi_m}}{\sqrt{\pi \cdot 25}} \cdot \frac{M}{1+M} \cdot \sum_{j=1}^{m-1} \left(\Psi_j \cdot S1_{m-j+1}\right) - \frac{\gamma}{1+M} \cdot e^{-(1-\alpha) \cdot \Phi_m} \cdot \sum_{j=1}^{m-1} \left(\Psi_j \cdot S_{m-j+1}\right)}{1 + \frac{0.04 \cdot w \cdot e^{\alpha \cdot \Phi_m} \cdot 1}{\sqrt{1 \cdot 1}} + \frac{2 \cdot K \cdot e^{-(1-\alpha) \cdot \Phi_m}}{\sqrt{\pi \cdot 25}} \cdot \frac{M}{1+M} + \frac{\gamma}{1+M} \cdot e^{-(1-\alpha) \cdot \Phi_m} \cdot S_1}$$

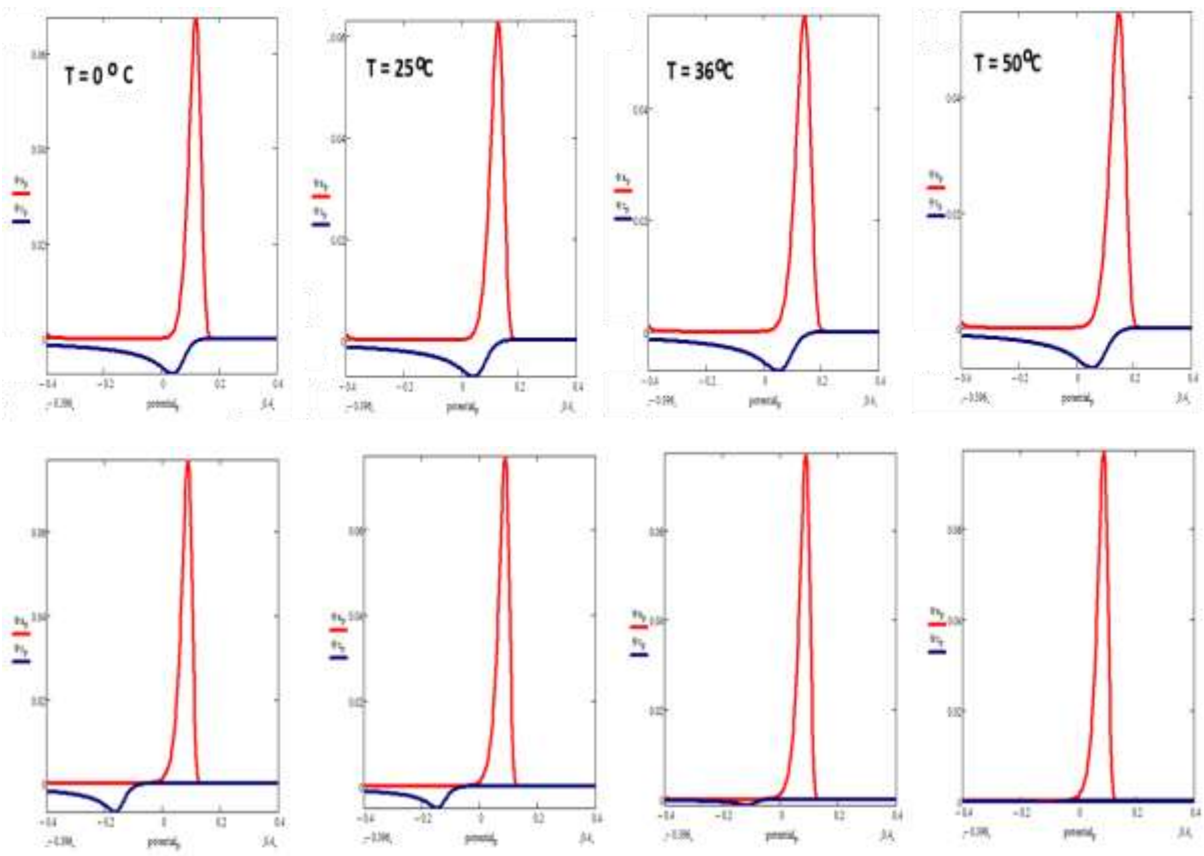
$$\Psi_n := \frac{w \cdot e^{\alpha \cdot b_n} - \frac{0.04 \cdot w \cdot e^{\alpha \cdot b_n}}{\sqrt{1 \cdot 1}} \cdot \sum_{j=1}^{n-1} \left(\Psi_j \cdot 1\right) - \frac{2 \cdot K \cdot e^{-(1-\alpha) \cdot b_n}}{\sqrt{\pi \cdot 25}} \cdot \frac{M}{1+M} \cdot \sum_{j=1}^{n-1} \left(\Psi_j \cdot S1_{n-j+1}\right) - \frac{\gamma}{1+M} \cdot e^{-(1-\alpha) \cdot b_n} \cdot \sum_{j=1}^{n-1} \left(\Psi_j \cdot S_{n-j+1}\right)}{1 + \frac{0.04 \cdot w \cdot e^{\alpha \cdot b_n} \cdot 1}{\sqrt{1 \cdot 1}} + \frac{2 \cdot K \cdot e^{-(1-\alpha) \cdot b_n}}{\sqrt{\pi \cdot 25}} \cdot \frac{M}{1+M} + \frac{\gamma}{1+M} \cdot e^{-(1-\alpha) \cdot b_n} \cdot S_1}$$

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





Effect of concentration of the system that interacts with the metallic dental biomaterial (cyclic voltammograms at the end of the potential window show increase in the current)



Effect of the rate of coupled chemical reaction to the features of voltammograms representing Dissolution of dental material in physiological conditions

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