MATHCAD платформа за симулации на EC' дифузиски регенеративен механизам во циклична волтаметрија

Rubin Gulaboski

Faculty of Medical Sciences, Goce Delcev University, Stip, Macedonia

Abstract: Претставен е MATHCAD протокол за симулирање на електрохемиски регенеративен дифузиски механизам во услови на циклична волтаметрија. Механизмот е соодветен за објаснување на електрохемиските својства на редокс протеини што се растворливи во вода. Фајлот е даден во слободна форма и е достапен за симулирање со аплицирање во MATHCAD симулацискиот пакет.

Ciklicna skalesta voltametrija

DIFFUSIONAL EC' MECHANISM
in CYCLIC STAIRCASE VOLTAMMETRY

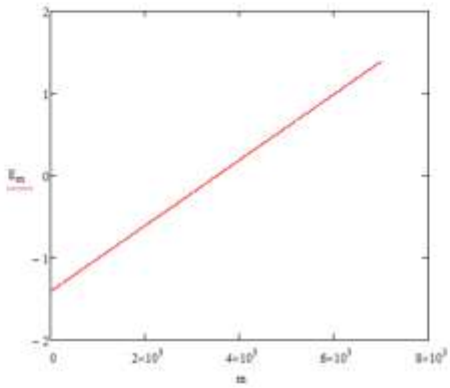
$tac := 0.02$

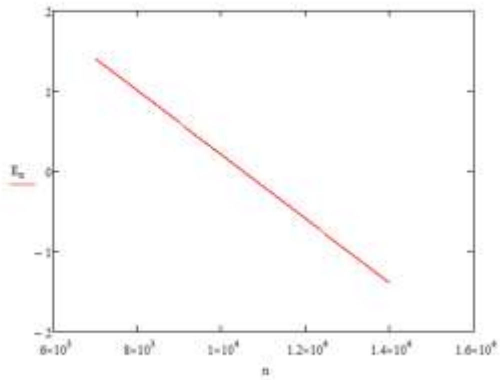
$Es := -1.4 \quad Ef := 1.4 \quad \Delta E := Ef - Es \quad dE := 0.01 \quad \tau := 0.05 \quad d := \frac{\tau}{25} \quad s := 1 .. \frac{tac}{d}$

$m := \frac{tac}{d} + 1 .. \frac{\Delta E}{dE} \cdot 25 + \frac{tac}{d} \qquad n := \frac{\Delta E}{dE} \cdot 25 + \frac{tac}{d} + 1 .. \left(\frac{\Delta E}{dE} \cdot 25 \cdot 2 + \frac{tac}{d}\right) \qquad \frac{\Delta E}{dE} = 280$

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

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





$\Lambda := 0.28 \qquad cox := 0.0000008$

$ks := .000000245 \qquad D := 3\cdot10^{-6}$

$\lambda := \frac{ks\cdot\sqrt{\tau}}{} \qquad \alpha := 0.5$

$\lambda = 3.163 \times 10^{-5}$

$\log(\lambda) = -4.5 \qquad kc := 10^{.2597042030272005205242}$ -konstan na kataliza

1

$z := (kc\cdot\tau)$

$F := 96500 \quad el := 1 \quad R := 8.314 \quad T := 298.15$

$\Phi_m := el \cdot \frac{F}{R \cdot T} \cdot (E_m) \quad b_n := el \cdot \frac{F}{R \cdot T} \cdot (E_n) \qquad \Phi ac := el \cdot \frac{F}{R \cdot T} \cdot Es$

$z = 0.091 \qquad \frac{\lambda}{z} = 3.479 \times 10^{-4}$

$\log(z) = -1.041 \qquad \frac{z}{\lambda} = 2.875 \times 10^{3}$

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

ova S1 ne treba za ovoj EC' mehanizam

$S1_k := \sqrt{k} - \sqrt{k-1}$

$S_k := \left(1 - \mathrm{erfc}\left(\sqrt{\frac{z}{25 \times 1} \cdot k}\right)\right) - \left[1 - \mathrm{erfc}\left[\sqrt{\frac{z}{25 \times 1} \cdot (k-1)}\right]\right]$

$$S_1 = 0.068$$

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

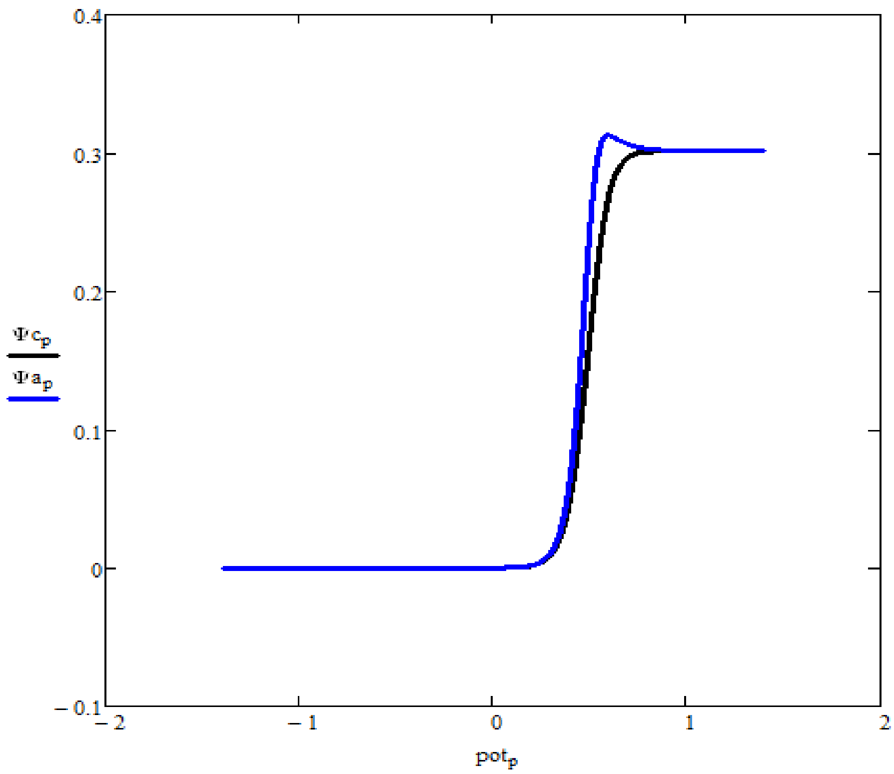
$$\Psi_1 = 3.163 \times 10^{-5}$$

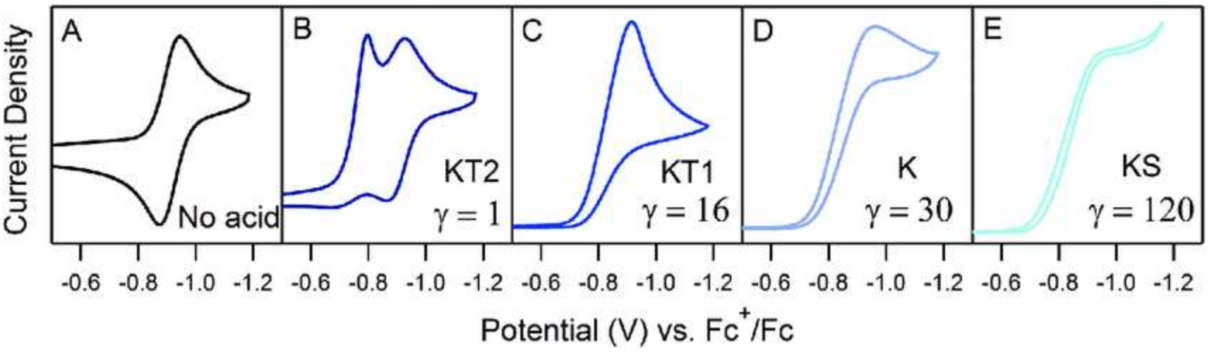
$$\Psi_s := \frac{\lambda \cdot e^{\alpha \cdot \Phi ac} - \frac{\lambda \cdot e^{\alpha \cdot \Phi ac}}{\sqrt{1z}} \cdot \sum_{j=1}^{s-1} \left(\Psi_j \cdot S_{s-j+1} \right) - e^{-\Phi ac \cdot (1-\alpha)} \cdot \lambda \cdot \frac{1}{\sqrt{1z}} \cdot \sum_{j=1}^{s-1} \left(\Psi_j \cdot S_{s-j+1} \right)}{1 + \frac{\lambda \cdot e^{\alpha \cdot \Phi ac} \cdot S_1}{\sqrt{1z}} + \frac{\lambda \cdot e^{-(1-\alpha)\cdot \Phi ac} \cdot S_1}{\sqrt{1z}}}$$

$$\Psi_m := \frac{\lambda \cdot e^{\alpha \cdot \Phi_m} - \frac{\lambda \cdot e^{\alpha \cdot \Phi_m}}{\sqrt{1z}} \cdot \sum_{j=1}^{m-1} \left(\Psi_j \cdot S_{m-j+1} \right) - e^{-\Phi_m \cdot (1-\alpha)} \cdot \lambda \cdot \frac{1}{\sqrt{1z}} \cdot \sum_{j=1}^{m-1} \left(\Psi_j \cdot S_{m-j+1} \right)}{1 + \frac{\lambda \cdot e^{\alpha \cdot \Phi_m} \cdot S_1}{\sqrt{1z}} + \frac{\lambda \cdot e^{-(1-\alpha)\cdot \Phi_m} \cdot S_1}{\sqrt{1z}}}$$

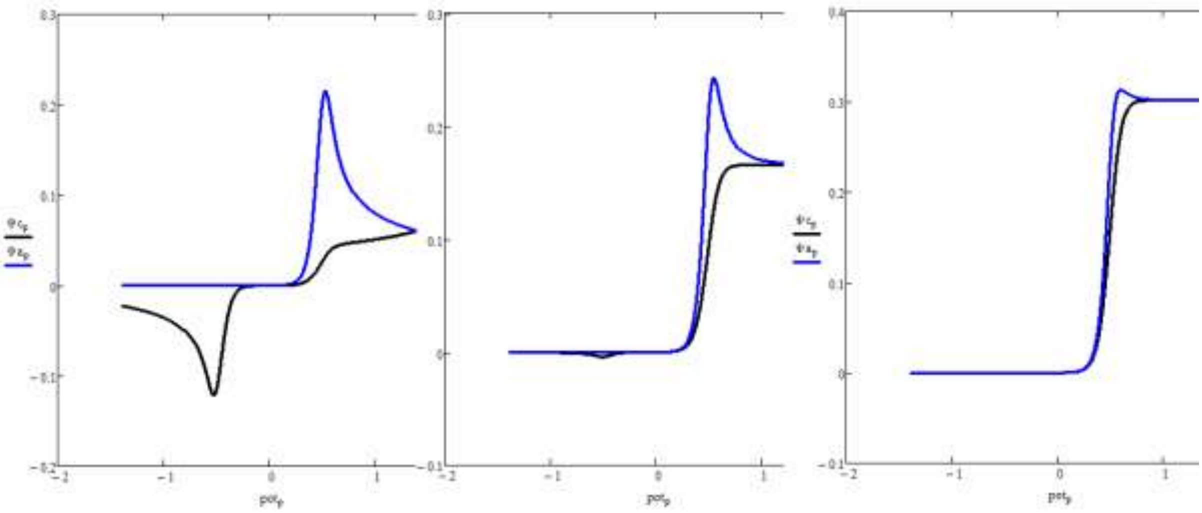
$$\Psi_n := \frac{\lambda \cdot e^{\alpha \cdot b_n} - \frac{\lambda \cdot e^{\alpha \cdot b_n}}{\sqrt{1z}} \cdot \sum_{j=1}^{n-1} \left(\Psi_j \cdot S_{n-j+1} \right) - e^{-b_n \cdot (1-\alpha)} \cdot \lambda \cdot \frac{1}{\sqrt{1z}} \cdot \sum_{j=1}^{n-1} \left(\Psi_j \cdot S_{n-j+1} \right)}{1 + \frac{\lambda \cdot e^{\alpha \cdot b_n} \cdot S_1}{\sqrt{1z}} + \frac{\lambda \cdot e^{-(1-\alpha)\cdot b_n} \cdot S_1}{\sqrt{1z}}}$$

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





Влијание на константата на регенеративна хемиска реакција врз цикличните одговори во голем распон на брзини на регенеративната реакција кај реверзибилна електродна реакција



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LITERATURE

1. R. Gulaboski, ***Journal of Solid State Electrochemistry*** 24 (**2020**) 2081-2081
2. R. Gulaboski, E. S. Ferreira, C. M. Pereira, M. N. D. S. Cordeiro, A. Garau, V. Lippolis, A. F. Silva, ***Journal of Physical Chemistry C*** 112 (2008) 153-161
3. R. Gulaboski, V. Mirceski, M. Lovric, I. Bogeski, ***Electrochemistry Communications*** 7 (2005) 515-522.
4. R Gulaboski, V Mirceski, ***Macedonian Journal of Chemistry and Chemical Engineering*** 39 (2020) 153-166
5. V. Mirceski, R. Gulaboski, ***Macedonian Journal of Chemistry and Chemical Engineering*** 33 (2014), 1-12
6. V. Mirceski, R. Gulaboski, ***Journal of Solid State Electrochemistry*** 7 (2003) 157-165
7. M. Janeva, P. Kokoskarova, V. Maksimova, R. Gulaboski, ***Electroanalysis*** 31 (2019) 2488-2506
8. R. Gulaboski, V. Mirceski, S. Komorsky-Lovric, M. Lovric, ***Electroanalysis*** 16 (2004) 832-842
9. R. Gulaboski, C.M. Pereira, M.N.D.S Cordeiro, I. Bogeski, F. Silva, ***Journal of Solid State Electrochemistry,*** 9, **2005**, 469-474
10. B. Sefer, R. Gulaboski, V. Mirceski, ***Journal of Solid State Electrochemistry*** 16 (2012) 2373-2381.
11. V. Mirceski, R. Gulaboski, ***Bulletin of the Chemists and Technologists of Macedonia*** 18 (1999) 57-64.
12. R. Gulaboski, C. M. Pereira, ***Electroanalytical Techniques and Instrumentation in Food Analysis***; in Handbook of Food Analysis Instruments (2008) 379-402.
13. M. Jorge, R. Gulaboski, C. M. Pereira, M. N. D. S. Cordeiro, ***Journal of Physical Chemistry B*** 110 (2006) 12530-12538.
14. V. Mirceski, D. Guziejewski, L. Stojanov, R. Gulaboski, ***Analytical Chemistry*** 91 (2019) 14904-14910.
15. V. Mirceski, R. Gulaboski, F. Scholz, ***Journal of Electroanalytical Chemistry*** 566 (2004) 351-360.

16. R. Gulaboski, M. Chirea, C. M. Pereira, M. N. D. S. Cordeiro, R. B. Costa, A. F. Silva, ***J. Phys. Chem. C*** 112 (2008) 2428-2435

17. R. Gulaboski, V. Mirceski, S. Komorsky-Lovric, M. Lovric, ***Electroanalysis*** 16 (2004) 832-842

18. R. Gulaboski, C. M. Pereira, M. N. D. S. Cordeiro, A. F. Silva, M. Hoth, I. Bogeski, ***Cell Calcium*** 43 (2008) 615-621

19. R. Gulaboski, V. Mirceski, F. Scholz, ***Amino Acids*** 24 (2003) 149-154

20. V. Mirceski, R. Gulaboski, ***Croatica Chemica Acta*** 76 (2003) 37-48.

21. F. Scholz, R. Gulaboski, ***Faraday Discussions*** 129 (2005) 169-177.

22. R. Gulaboski, K. Caban. Z. Stojek, F. Scholz, ***Electrochemistry Communications*** 6 (2004) 215-218.

23. V. Mirceski, R. Gulaboski, ***Journal of Physical Chemistry B***, 110 (2006) 2812-2820.

24. V. Mirceski, R. Gulaboski, B. Jordanoski, S. Komorsky-Lovric, ***Journal of Electroanalytical Chemistry,*** 490 (2000) 37-47.

25. R. Gulaboski, ***Macedonian Journal of Chemistry and Chemical Engineering*** 41 (2022) 151-162

26. R. Gulaboski, P. Kokoskarova, S. Petkovska, ***Analytical&Bioanalytical Electrochemistry***, 12 (2020) 345-364.

27. V. Mirčeski, R. Gulaboski, F. Scholz, ***Electrochemistry Communications*** 4 (10) **2002**, 814-819

28. M. Jorge, R. Gulaboski, C. M. Pereira, M. N. D. S Cordeiro, ***Molecular Physics*** 104 (2006) 3627-3634.

29. R. Gulaboski, V. Mirceski, M. Lovric, ***Macedonian Journal of Chemistry and Chemical Engineering*** 40 (2021) 1-9.

30. R. Gulaboski, P. Kokoskarova, S. Risafova, ***J. Electroanal. Chem***. 868 (2020) 114189.

31. R. Gulaboski, V. Mirceski, ***Journal of Solid State Electrochemistry*** 28 (2024) 1121-1130.

32. V. Mirceski, B. Mitrova, V. Ivanovski, N. MItreska, A. Aleksovska, R. Gulaboski, ***Journal of Solid State Electrochemistry*** 19 (2015) 1121-1130.

33. I. Spirevska, L. Soptrajanova, R. Gulaboski, **Analytical Letters** 33 (2000) 919-928.