

Class Project

Due: Friday, April 22nd

In this project, you will use computer simulations to determine cyclic voltammetric i-E curve shapes as a function of k^0 , α , analyte concentration, and redox reaction mechanism. The software you will use is DigiSim 3.1 and it is available on a computer in room 306 of the Chemistry Building.

You will need to save the curves you generate and eventually print them out with a short summary. You will have to determine E_{init} and E_{final} for the simulations.

1. For the redox reaction, $O + e = R$, and $E^0 = 0.250 \text{ V}$, $C_{\text{ox}} = 1 \text{ mM}$, $D = 5 \times 10^{-6} \text{ cm}^2/\text{s}$ and $\alpha=0.5$, determine how the curve shapes change as a function of scan rate (0.1, 0.2, 0.3, 0.4 and 0.5 V/s) with $k^0 = 10^{-2}$, 10^{-3} , 10^{-4} and 10^{-5} cm/s . What are the ΔE_p and i_p^{red} values with scan rate and rate constant? Assume that only C_{ox} is present to begin with. Do not add any R_{ohmic} or C_{dl} values to the simulation.
2. For the same redox reaction and conditions, determine how the curve shapes change as a function of scan rate (0.1, 0.2, 0.3, 0.4 and 0.5 V/s) for $k^0=10^{-3} \text{ cm/s}$ when R_{ohmic} is changed from 10, 100, 500 and 1000 ohms. What are the ΔE_p and i_p^{red} values with scan rate and rate constant? Assume that only C_{ox} is present to begin with.
3. For the same redox reaction and conditions, determine how the curve shapes change as a function of scan rate (0.1, 0.2, 0.3, 0.4 and 0.5 V/s) for $k^0=10^{-3} \text{ cm/s}$ when C_{dl} is changed from 10, 45, 75 and 100 $\mu\text{F}/\text{cm}^2$. What are the ΔE_p and i_p^{red} values with scan rate and rate constant? Assume that only C_{ox} is present to begin with.
4. For the redox reaction, $O + e = R$, and $E^0 = 0.250 \text{ V}$, $D = 5 \times 10^{-6} \text{ cm}^2/\text{s}$ and $\alpha=0.5$, determine how the curve shapes change at 0.1 V/s with $k^0 = 10^{-2}$, 10^{-3} , 10^{-4} and 10^{-5} cm/s and $C_{\text{ox}} = 0.1$, 0.5 and 1 mM. What are the ΔE_p and i_p^{red} values with scan rate and rate constant? Assume that only C_{ox} is present to begin with. Do not add any R_{ohmic} or C_{dl} values to the simulation.
5. Determine how the background voltammetric curves change shape and current magnitude with scan rate between 0.5 and -0.5 V for $C_{\text{dl}} = 10 \mu\text{F}/\text{cm}^2$ and $R_{\text{ohmic}} = 10$, 100, 500 and 1000 ohms, and for $C_{\text{dl}} = 100 \mu\text{F}/\text{cm}^2$ at the same R_{ohmic} values.