

Toolbox terminology

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1 Chronoamperometry

1.1 What is Chronoamperometry?

Chronoamperometry is an electrochemical technique where a constant potential is applied to an electrode, and the resulting current is measured as a function of time. This technique is used to study the kinetics of electrochemical reactions, diffusion processes, and the stability of electrode materials.

1.2 Principle of Chronoamperometry

In chronoamperometry, a potential step is applied to the working electrode, and the resulting current decay is monitored. The initial current spike is due to the rapid charging of the electrical double layer and the immediate electrochemical reaction. Over time, the current decreases as the concentration of the electroactive species near the electrode surface is depleted and diffusion controls the rate of the reaction.

1.3 Equation

The current response in chronoamperometry for a diffusion-controlled process is described by the Cottrell equation:

$$i(t) = \frac{nFAC^*D^{1/2}}{\pi^{1/2}t^{1/2}} \quad (1)$$

Where:

- $i(t)$ = Current at time t (A)
- n = Number of electrons transferred in the reaction
- F = Faraday constant (96485 C/mol)
- A = Electrode area (cm²)
- c^* = Bulk concentration of the electroactive species (mol/cm³)
- D = Diffusion coefficient (cm²/s)
- t = Time (s)

1.4 Usage of Chronoamperometry

Chronoamperometry is used in various applications, including:

- **Diffusion Coefficients:** To measure the diffusion coefficients of electroactive species.
- **Material Characterization:** To study the stability and performance of electrode materials.
- **Electrodeposition:** To control the thickness and uniformity of electroplated films.

2 Cycle Range Parameter

2.1 What is it?

The **Cycle Range** parameter specifies the range of cycles (or scan numbers) that the software will analyze in a cyclic voltammetry (CV) experiment. This parameter allows you to focus on a specific subset of the overall data, excluding the initial or final cycles that may not represent the steady-state behavior of the system.

2.2 How to set?

You can set this parameter by defining the starting and ending cycle numbers that you want to include in the analysis. This is particularly useful when the initial cycles may contain artifacts or the final cycles may show signs of degradation or instability.

Example: If you want to analyze cycles 2 through 15, you would set the Cycle Range as `range(2, 16)`. This means the software will analyze from the second cycle up to, but not including, the 16th cycle (so cycles 2 to 15).

This flexibility allows you to tailor the analysis to the specific regions of the data that are most relevant to your research objectives, ensuring that the analysis is focused and accurate.

3 Discard Scan Rate Parameters

3.1 What It Is?

The “**Discard scan rate from**” and “**Discard scan rate after**” parameters allow you to exclude specific scans from the beginning and end of your dataset before conducting analysis. These parameters are particularly useful in ensuring that your analysis focuses only on the most relevant and accurate data, avoiding any potential artifacts or inconsistencies in the initial and final scans.

- **Discard scan rate from:** This parameter specifies the number of scans to discard from the start of the dataset.
- **Discard scan rate after:** This parameter specifies the number of scans to discard from the end of the dataset.

These settings are especially useful when analyzing multiple peaks within your data. Different peaks might require different scan rate ranges to be accurately distinguished, and these parameters allow you to fine-tune the dataset to focus on specific regions of interest.

3.2 How to Set?

You can set these parameters based on your experimental needs, such as the behavior of the peaks and the conditions under which the scans were obtained.

Example:

- **Your dataset:**

- CV_data_10mVs
- CV_data_20mVs
- CV_data_50mVs
- CV_data_100mVs
- CV_data_150mVs
- CV_data_200mVs

- **Settings:**

- **Discard scan rate from:** [(1)]
- **Discard scan rate after:** [(1)]

- **Resulting Dataset After Discarding:**

- The scans that will be used for analysis are:
 - * CV_data_20mVs
 - * CV_data_50mVs
 - * CV_data_100mVs
 - * CV_data_150mVs

Analyzing Multiple Peaks:

If your analysis involves multiple peaks, you can set the “**Discard scan rate from**” and “**Discard scan rate after**” parameters individually for each peak (for example: Discard scan rate from [(1, 0, 1)], Discard scan rate after [(1, 1, 0)], this indicates that you have three peaks to analyze. For peak 1: Analysis includes scans between the first and last, excluding those two. For peak 2: Analysis includes all scans except the last one. For peak 3: Analysis includes all scans except the first one.). This allows you to discard the scans that might interfere with the accurate identification of specific peaks. For instance, one peak might require excluding certain low scan rates to prevent overlap with another peak, while another peak might benefit from a different range of scan rates.

3.3 Why This Matters?

As the scan rate changes, the current peaks in your dataset may shift, causing them to merge with other peaks or become less visible. This can lead to inaccurate or misleading results. By carefully selecting which scans to include in your analysis—specifically by discarding the initial and final scans that might introduce errors—you can ensure that each peak remains distinct and that your analysis is more accurate.

When analyzing multiple peaks, adjusting the scan rates for each peak helps prevent overlap, ensuring that each peak is analyzed within the most appropriate range. This improves the precision of your results and leads to more reliable conclusions in your study.

4 Diffusion Coefficient (D)

4.1 What is the Diffusion Coefficient?

The **diffusion coefficient**, denoted as D , is a measure of the rate at which particles or molecules spread out or diffuse through a medium. It is typically expressed in units of square centimeters per second (cm^2/s) or square meters per second (m^2/s). The diffusion coefficient is an important parameter in describing the kinetics of diffusion-controlled processes.

4.2 Example

Consider a solute with a diffusion coefficient of $1 \times 10^{-5} \text{ cm}^2/\text{s}$ in a solution. This means that, on average, the solute molecules will diffuse through the solvent at a rate of 1×10^{-5} square centimeters per second. The higher the diffusion coefficient, the faster the molecules move through the medium.

4.3 Usage

The diffusion coefficient (D) is used in various contexts, including:

- **Fick's Laws of Diffusion:** To describe the flux and concentration gradients in a system.
- **Electrochemical Analysis:** To determine the rate of mass transport in electrochemical cells.
- **Material Science:** To study the diffusion of atoms and molecules in solids and liquids.
- **Environmental Science:** To model the dispersion of pollutants in air, water, and soil.

5 Initial Concentration (C_0)

5.1 What is Initial Concentration?

The **initial concentration**, denoted as C_0 , refers to the concentration of a substance in a solution at the beginning of an experiment or reaction. It is typically measured in moles per cubic centimeter (mol/cm^3) or moles per liter (M).

6 Kinematic Viscosity

6.1 What is Kinematic Viscosity?

Kinematic viscosity (ν) is a measure of a fluid's resistance to flow under the influence of gravity. It is defined as the ratio of the dynamic viscosity (μ) to the density (ρ) of the fluid. Kinematic viscosity is typically expressed in units of square meters per second (m^2/s) or Stokes (St), where $1 \text{ St} = 10^{-4} \text{ m}^2/\text{s}$.

6.2 Equation

The kinematic viscosity (ν) can be calculated using the following equation:

$$\nu = \frac{\mu}{\rho} \quad (2)$$

Where:

- ν = Kinematic viscosity (m^2/s)
- μ = Dynamic viscosity (Pa·s or kg/(m·s))
- ρ = Density of the fluid (kg/m^3)

6.3 Viscosity of Common Liquids

The table below lists the kinematic and dynamic viscosities of some common liquids at standard conditions (typically 20°C or 25°C).

Liquid	Dynamic Viscosity (μ) (Pa·s)	Density (ρ) (kg/m^3)	Kinematic Viscosity (ν) (m^2/s)
Water (20°C)	1.002×10^{-3}	998	1.004×10^{-6}
Ethanol (20°C)	1.074×10^{-3}	789	1.361×10^{-6}
Glycerol (20°C)	1.49	1260	1.183×10^{-3}
Mercury (25°C)	1.526×10^{-3}	13534	1.127×10^{-7}
Olive Oil (25°C)	8.1×10^{-2}	918	8.82×10^{-5}
Honey (25°C)	2 - 10	1400	1.43×10^{-3} to 7.14×10^{-3}

Table 1: Dynamic and Kinematic Viscosity of Common Liquids

7 Levich and Koutecky-Levich Analysis

7.1 What is Levich Analysis?

Levich Equation: The Levich equation describes the relationship between the limiting current and the rotation speed of a rotating disk electrode (RDE) in an electrochemical cell. It is used to determine the diffusion coefficient of the reacting species and the kinetics of the reaction.

$$I_L = 0.62nFAD^{2/3}\nu^{-1/6}\omega^{1/2}C \quad (3)$$

Where:

- I_L = Limiting current (A)
- n = Number of electrons transferred in the reaction
- F = Faraday constant (96485 C/mol)
- A = Electrode area (cm²)
- D = Diffusion coefficient (cm²/s)
- ν = Kinematic viscosity of the solution (cm²/s)
- ω = Angular rotation speed (rad/s)
- C = Concentration of the reactant (mol/cm³)

Usage:

- **Determining Diffusion Coefficient:** By measuring the limiting current at different rotation speeds, the diffusion coefficient D can be calculated.
- **Understanding Mass Transport:** It provides insights into how mass transport influences the overall reaction rate.

Example: If you have a series of limiting current values measured at different rotation speeds, you can plot I_L versus $\omega^{1/2}$. The slope of the resulting line can be used to determine the diffusion coefficient of the reactant.

7.2 What is Koutecky-Levich Analysis?

Koutecky-Levich Equation: The Koutecky-Levich equation combines the kinetics of the electron transfer process with the mass transport limitation to provide a comprehensive understanding of the reaction mechanism.

$$\frac{1}{I} = \frac{1}{I_k} + \frac{1}{I_L} \quad (4)$$

Where:

- I = Measured current (A)
- I_k = Kinetic current (A)
- I_L = Levich (diffusion-limited) current (A)

The kinetic current I_k is given by:

$$I_k = nFkAC \quad (5)$$

Where:

- k = Rate constant of the reaction (cm/s)

Usage:

- **Separating Kinetic and Diffusion Effects:** By measuring the current at different rotation speeds and applying the Koutecky-Levich equation, the kinetic current I_k can be separated from the diffusion-limited current I_L .
- **Determining Kinetic Parameters:** It helps in determining the rate constant k and understanding the intrinsic kinetics of the electrochemical reaction.

Example: If you plot $\frac{1}{I}$ versus $\frac{1}{\omega^{1/2}}$, you will get a straight line. The intercept gives $\frac{1}{I_k}$ (the inverse of the kinetic current), and the slope provides $\frac{1}{I_L}$ (the inverse of the Levich current).

7.3 How to Use Levich and Koutecky-Levich Analysis

1. **Perform RDE Experiments:** Conduct experiments at various rotation speeds to measure the limiting current I_L .
2. **Plot Levich Plot:** Plot the limiting current I_L against the square root of the rotation speed $\omega^{1/2}$.
3. **Determine Diffusion Coefficient:** From the slope of the Levich plot, calculate the diffusion coefficient D .
4. **Apply Koutecky-Levich Equation:** Use the Koutecky-Levich equation to separate the kinetic and diffusion contributions.
5. **Plot Koutecky-Levich Plot:** Plot $\frac{1}{I}$ versus $\frac{1}{\omega^{1/2}}$ to determine the kinetic current I_k and the rate constant k .

7.4 Examples in Practice

Levich Analysis Example: Suppose you measure the limiting current I_L at different rotation speeds:

- $\omega_1 = 100$ rad/s, $I_{L1} = 0.5$ A
- $\omega_2 = 400$ rad/s, $I_{L2} = 1.0$ A
- $\omega_3 = 900$ rad/s, $I_{L3} = 1.5$ A

Plotting I_L versus $\omega^{1/2}$ gives a straight line. From the slope, you can calculate the diffusion coefficient D .

Koutecky-Levich Analysis Example: Using the same data, plot $\frac{1}{I}$ versus $\frac{1}{\omega^{1/2}}$. The intercept gives $\frac{1}{I_k}$, and the slope provides $\frac{1}{I_L}$. From this plot, you can determine the kinetic parameters of the reaction.

By combining these analyses, you gain a deeper understanding of both the mass transport and kinetic aspects of your electrochemical reaction.

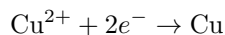
8 Number of Electron Transfer (n)

8.1 What is the Number of Electron Transfer?

The **number of electron transfer**, denoted as n , refers to the number of electrons involved in an electrochemical reaction. It is a key parameter in determining the stoichiometry of the reaction and is used in various electrochemical equations to describe the process.

8.2 Example

In the reduction of copper ions:



$n = 2$, indicating that two electrons are involved in the reduction of one copper ion.

9 Peak Range Parameters

9.1 What is it?

- **Peak Range (Top):** This parameter specifies the potential (voltage) ranges in the cyclic voltammogram where the software will search for peaks in the upper (positive) direction. Each pair of numbers represents a range of applied potentials (in volts) where a peak might occur in the positive direction.
- **Peak Range (Bottom):** This parameter is similar to the "Peak Range (Top)," but it specifies the potential ranges where the software will search for peaks in the lower (negative) direction. Each pair represents a range of potentials in the negative direction.

9.2 How to set?

You set these parameters by defining the potential ranges where you expect peaks to occur. When searching for peaks, it's crucial that the "Peak Range (Top)" and "Peak Range (Bottom)" parameters have the same number of pairs. This ensures that the software can correctly align and analyze peaks across both the positive and negative directions.

- **Single Peak Search:** $[(value_i, value_f)]$
If you want to search for just one peak, input a single pair of values specifying the potential range for both "Top" and "Bottom."
- **Multiple Peak Search:** $[(value_{1i}, value_{1f}), \dots, (value_{ni}, value_{nf})]$
If you expect to find multiple peaks, input multiple pairs of values, ensuring that the "Top" and "Bottom" parameters have the same length.

Example:

- **Single Peak Search:**

- If you're only interested in finding a peak between 0 V and 0.2 V in the positive direction, you would set the "Peak Range (Top)" as (0, 0.2) and the "Peak Range (Bottom)" similarly, say, (0, -0.2) if you expect a corresponding negative peak.

- **Multiple Peak Search:**

- Suppose you expect to find peaks within the ranges of -1 V to -0.70 V, 0 V to 0.2 V, and 0.25 V to 0.5 V. You would set the parameters as follows:

- * **Peak Range (Bottom):** (-1, -0.70), (0, -0.2), (0.25, -0.5)

- * **Peak Range (Top):** (-1, 0.70), (0, 0.2), (0.25, 0.5)

Here, both the "Top" and "Bottom" parameters include three pairs, ensuring that the software analyzes corresponding peaks in both directions.

By setting these ranges, the software will search for peaks within the specified voltage ranges in both the positive and negative directions, providing you with a comprehensive analysis of your cyclic voltammogram data.

10 Randles–Ševčík Analysis

10.1 What is Randles–Ševčík Analysis?

The **Randles–Ševčík analysis** is a method used in electrochemistry to analyze cyclic voltammetry data. It relates the peak current observed in a cyclic voltammogram to the scan rate, the concentration of the electroactive species, and the diffusion coefficient. This analysis is particularly useful for reversible electrochemical reactions.

10.2 Equation

The Randles–Ševčík equation for a reversible reaction at 25°C is given by:

$$i_p = (2.69 \times 10^5) n^{3/2} A D^{1/2} C \nu^{1/2} \quad (6)$$

Where:

- i_p = Peak current (A)
- n = Number of electrons transferred in the redox event
- A = Electrode area (cm²)
- D = Diffusion coefficient (cm²/s)
- C = Concentration of the electroactive species (mol/cm³)
- ν = Scan rate (V/s)

10.3 Usage of Randles–Ševčík Analysis

Randles–Ševčík analysis is commonly used to:

- Determine the diffusion coefficient of the electroactive species.
- Analyze the kinetics of the electrochemical reaction.
- Investigate the reversibility of the electrochemical process.

10.4 How to Use Randles–Ševčík Analysis

1. **Perform Cyclic Voltammetry (CV) Experiments:** - Conduct CV experiments at various scan rates (ν) to measure the peak current (i_p).
2. **Plot Peak Current vs. Scan Rate:** - Plot the peak current (i_p) against the square root of the scan rate ($\nu^{1/2}$).
3. **Determine Diffusion Coefficient:** - The slope of the resulting linear plot can be used to determine the diffusion coefficient (D) using the Randles–Ševčík equation.

10.5 Example in Practice

Example: Suppose you perform CV experiments for a redox couple with the following parameters:

- $n = 1$ (one-electron transfer)
- $A = 0.1 \text{ cm}^2$ (electrode area)
- $C = 1 \times 10^{-3} \text{ mol/cm}^3$ (concentration)
- $\nu = 0.01$ to 0.1 V/s (scan rate range)

By plotting the peak current (i_p) versus the square root of the scan rate ($\nu^{1/2}$), you obtain a straight line. The slope of this line (s) is related to the diffusion coefficient (D) by the Randles–Ševčík equation:

$$s = 2.69 \times 10^5 n^{3/2} A D^{1/2} C$$

From the slope, you can solve for the diffusion coefficient D .

11 Rate Constant (k)

11.1 What is the Rate Constant?

The **rate constant**, denoted as k , is a proportionality constant in the rate equation of a chemical reaction. It provides a measure of the speed at which a reaction occurs. The rate constant is specific to a given reaction at a particular temperature and is typically determined experimentally.

11.2 Example

For a first-order reaction:

$$\text{Rate} = k[A]$$

where $[A]$ is the concentration of the reactant. The rate constant k has units of s^{-1} .

For a second-order reaction:

$$\text{Rate} = k[A][B]$$

where $[A]$ and $[B]$ are the concentrations of the reactants. The rate constant k has units of $\text{M}^{-1}\text{s}^{-1}$.

11.3 Usage

The rate constant (k) is used in various contexts, including:

- **Determining Reaction Rates:** To calculate the speed of a reaction based on reactant concentrations.
- **Comparing Reactions:** To compare the reactivity of different reactions under similar conditions.
- **Kinetic Studies:** To analyze the effect of different parameters, such as temperature and catalysts, on the reaction rate.

12 Smoothed/Smoothing Level (σ)

12.1 What is Smoothed/Smoothing Level (σ)?

The term **Smoothed/Smoothing Level (σ)** refers to a parameter used in various data analysis and signal processing techniques to reduce noise and smooth out fluctuations in data. The smoothing level is often represented by the Greek letter σ , which indicates the standard deviation of the Gaussian kernel used in the smoothing process.

12.2 Usage of Smoothing Level (σ)

Smoothing is commonly applied in the following contexts:

- **Data Analysis:** To reveal underlying trends in data by reducing random fluctuations.
- **Signal Processing:** To filter out high-frequency noise from signals.
- **Image Processing:** To blur images and reduce detail or noise.

12.3 How to Use Smoothing Level (σ)

Choosing σ : - The value of σ determines the degree of smoothing. **A larger σ results in more smoothing, while a smaller σ preserves more detail.** - The appropriate σ value depends on the specific application and the nature of the data. - The default value is often set to 10, but it should be adjusted based on the desired smoothing effect.

13 Surface Area (A)

13.1 What is Surface Area?

The **surface area**, denoted as A , refers to the area of the electrode that is in contact with the electrolyte in an electrochemical cell. It is typically measured in square centimeters (cm^2).

14 Tafel Analysis

14.1 What is Tafel Analysis?

The **Tafel analysis** is a method used in electrochemistry to determine the kinetics of an electrochemical reaction. It involves analyzing the Tafel plot, which is a plot of the logarithm of the current density ($\log j$) versus the overpotential (η). The Tafel equation describes the relationship between the overpotential and the current density, providing insights into the reaction mechanism and the rate-determining step.

14.2 Tafel Equation

The Tafel equation for an anodic reaction is given by:

$$\eta = a + b \log j \quad (7)$$

Where:

- η = Overpotential (V)
- j = Current density (A/cm^2)
- a = Tafel intercept (V)
- b = Tafel slope (V/decade)

For a cathodic reaction, the Tafel equation is:

$$\eta = a - b \log j \quad (8)$$

14.3 Usage of Tafel Analysis

Tafel analysis is commonly used to:

- Determine the Tafel slope, which provides information about the rate-determining step of the reaction.
- Calculate the exchange current density, which is related to the intrinsic kinetics of the reaction.
- Evaluate the efficiency of electrocatalysts.

14.4 How to Use Tafel Analysis

1. **Perform Electrochemical Measurements:** - Conduct experiments to measure the current density (j) at various overpotentials (η).
2. **Plot the Tafel Plot:** - Plot η versus $\log j$ to obtain the Tafel plot.
3. **Determine Tafel Parameters:** - From the linear region of the Tafel plot, determine the Tafel slope (b) and intercept (a).

14.5 Example in Practice

Example: Suppose you perform electrochemical measurements for a reaction and obtain the following data:

- $j = 1 \text{ mA/cm}^2$ at $\eta = 0.1 \text{ V}$
- $j = 10 \text{ mA/cm}^2$ at $\eta = 0.2 \text{ V}$
- $j = 100 \text{ mA/cm}^2$ at $\eta = 0.3 \text{ V}$

Plotting η versus $\log j$ yields a straight line. The Tafel slope (b) can be determined from the slope of this line, and the intercept (a) can be found from the y-intercept.