

Original Research

ELECTROCHEMICAL SENSING OF CAFFEINE

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Abstract

Caffeine is one of the most widely consumed psychoactive compounds and has gained increasing attention as an environmental and anthropogenic marker due to its frequent occurrence in wastewater and aquatic systems. Electrochemical methods have recently emerged as attractive alternatives for caffeine determination because of their simplicity, low cost, rapid response, and sensitivity. In this work, graphite pencil electrodes were investigated as renewable and economically accessible carbon-based electrodes for caffeine analysis in Britton–Robinson buffer using cyclic voltammetry. The electrochemical behavior of caffeine was investigated at different scan rates in order to evaluate the anodic response and oxidation characteristics of the system. In addition, Python-based data processing was applied for visualization, regression analysis, and automated interpretation of cyclic voltammetry data. The obtained results indicate predominantly irreversible electrochemical behavior of caffeine on graphite pencil electrodes with a significant dependence of anodic peak current on scan rate. The proposed approach demonstrates the potential of combining low-cost electrochemical sensing with open-source computational tools for electrochemical data analysis.

Keywords: caffeine, cyclic voltammetry, graphite pencil electrode, electrochemical analysis, Python.

INTRODUCTION

Caffeine (CAF) is a naturally occurring purine alkaloid widely present in coffee, tea, energy drinks, pharmaceuticals, and numerous consumer products. Due to its high consumption and continuous release into wastewater systems, caffeine has attracted significant attention as a biomarker and anthropogenic indicator of human activity and domestic wastewater contamination. Its presence in aquatic environments is frequently associated with urban pollution, wastewater discharge, and environmental monitoring studies, making caffeine an important target compound in analytical chemistry and environmental assessment [1–3].

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The increasing demand for rapid and accessible monitoring methods has stimulated the development of alternative analytical approaches for caffeine determination. Conventional methods such as chromatography and spectroscopic analysis provide high sensitivity and accuracy but often require expensive instrumentation, complex sample preparation, and specialized laboratory conditions. In recent years, electrochemical methods have become increasingly attractive due to their simplicity, rapid response, low operational cost, and suitability for real-time analysis [4–6].

Among various electrochemical sensing materials, carbon-based electrodes have gained particular importance because of their favorable electrochemical properties, chemical stability, and economic accessibility. Graphite pencil electrodes (PGE) represent a low-cost and renewable alternative to conventional solid electrodes, by removing the need for surface renewal and making the preparation process trivial in comparison with other electrodes, while being widely available [7–11].

In this work, cyclic voltammetry was employed for the investigation of caffeine oxidation behavior on graphite pencil electrodes in Britton–Robinson (BR) buffer at different scan rates. Furthermore, Python-based scientific computing and data processing tools were utilized for automated visualization, regression analysis, and interpretation of electrochemical data. The integration of low-cost electrochemical sensors with open-source computational methods represents a promising approach for reproducible and accessible electrochemical analysis [10–15].

MATERIALS AND METHODS

A caffeine solution with a concentration of $1 \cdot 10^{-3}$ M was prepared in Britton–Robinson (BR) buffer. Electrochemical measurements were performed using cyclic voltammetry (CV) in a three-electrode electrochemical system consisting of a graphite pencil electrode (PGE) as the working electrode (WE), a platinum wire as the counter electrode (CE), and a calomel electrode as the reference electrode (RE). HB graphite leads for mechanical pencils were used as graphite pencil electrodes. The electrochemical response of caffeine was investigated at scan rates of 20, 50, and 100 mV/s.

Graphite pencil electrodes (PGE) were selected due to their low cost and wide availability. Cyclic voltammetry measurements were carried out in order to evaluate the electrochemical behavior of caffeine and the influence of scan rate on the anodic response of the system.

Electrochemical data obtained from the IVIUM electrochemical workstation were exported in ASCII format and processed using Python-based scientific computing tools. A custom Python-based workflow was developed for electrochemical data interpretation and visualization of cyclic voltammetry measurements. Numerical processing and structured data handling were performed using NumPy and Pandas libraries, while SciPy was applied for regression analysis and peak-related data processing. Visualization of cyclic voltammetry curves and regression plots was performed using Matplotlib and PyQtGraph libraries. The complete experimental and computational workflow used in this study is presented in Figure 1 [4–6,8,9,12–15].

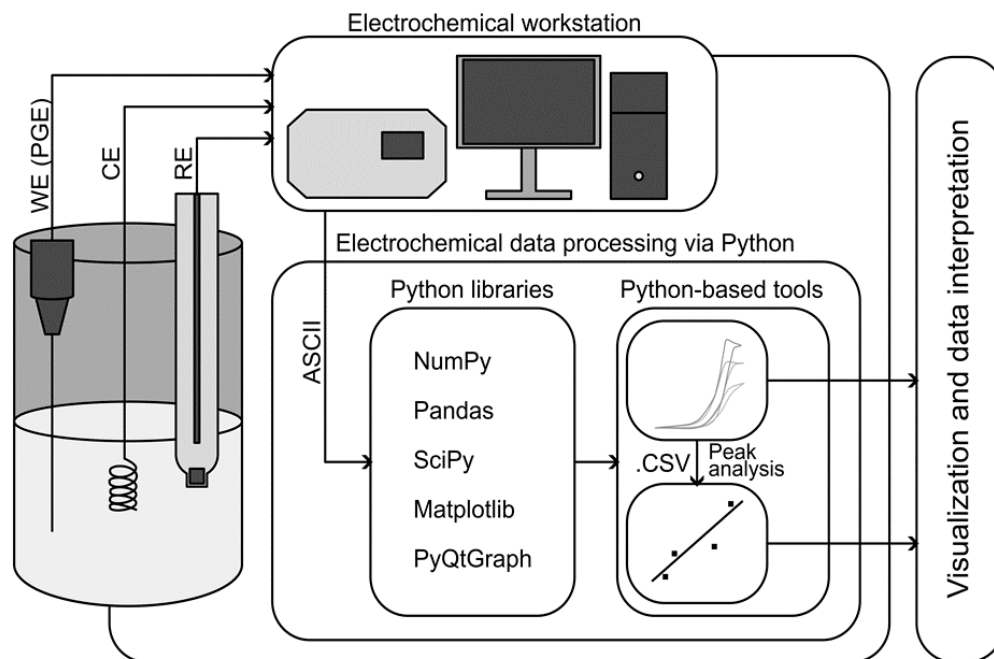


Figure 1 Schematic representation of the electrochemical and Python-assisted workflow used for cyclic voltammetry data acquisition, processing, regression analysis, and interpretation

RESULTS AND DISCUSSION

Figure 2 presents cyclic voltammograms obtained for $1 \cdot 10^{-3}$ M caffeine solution in BR buffer using a graphite pencil electrode at scan rates of 20, 50, and 100 mV/s, which are represented by blue, red, and green curves, respectively.

The obtained voltammograms show a pronounced anodic response in the high potential region, while no clearly defined cathodic counterpart was observed during the reverse scan, indicating predominantly irreversible electrochemical behavior of caffeine on the graphite pencil electrode surface. Similar electrochemical behavior of caffeine oxidation on carbon-based electrodes has been previously reported in the literature [10,16]. The observed oxidation region and voltammetric profile are also in agreement with previously described anodic oxidation mechanisms of caffeine in aqueous media [16]. The applicability of graphite pencil electrodes for caffeine oxidation in the high potential region may also be associated with the relatively wide anodic potential window and favorable electrochemical properties of graphite-based materials [11].

The anodic peak potential (E_p) was observed in the high potential region between approximately 1.58 and 1.62 V, while the anodic peak current (I_p) increased with increasing scan rate. The shift of E_p toward more positive potentials together with the increase of I_p at higher scan rates is characteristic of irreversible electrochemical oxidation processes and agrees with previously reported electrochemical behavior of caffeine on carbon-based electrodes [10,16]. According to the obtained results, the anodic peak current increased from 0.0275 mA at 20 mV/s to 0.1083 mA at 100 mV/s, while E_p shifted from 1.5860 to 1.6207 V. An increase in scan rate resulted in a significant increase in anodic current intensity together with noticeable changes in voltammetric profile and peak shape. At higher scan rates, the

existing anodic features became more pronounced, which is consistent with the oxidation of caffeine on heterogeneous graphite-based electrode surfaces [5,10,11].

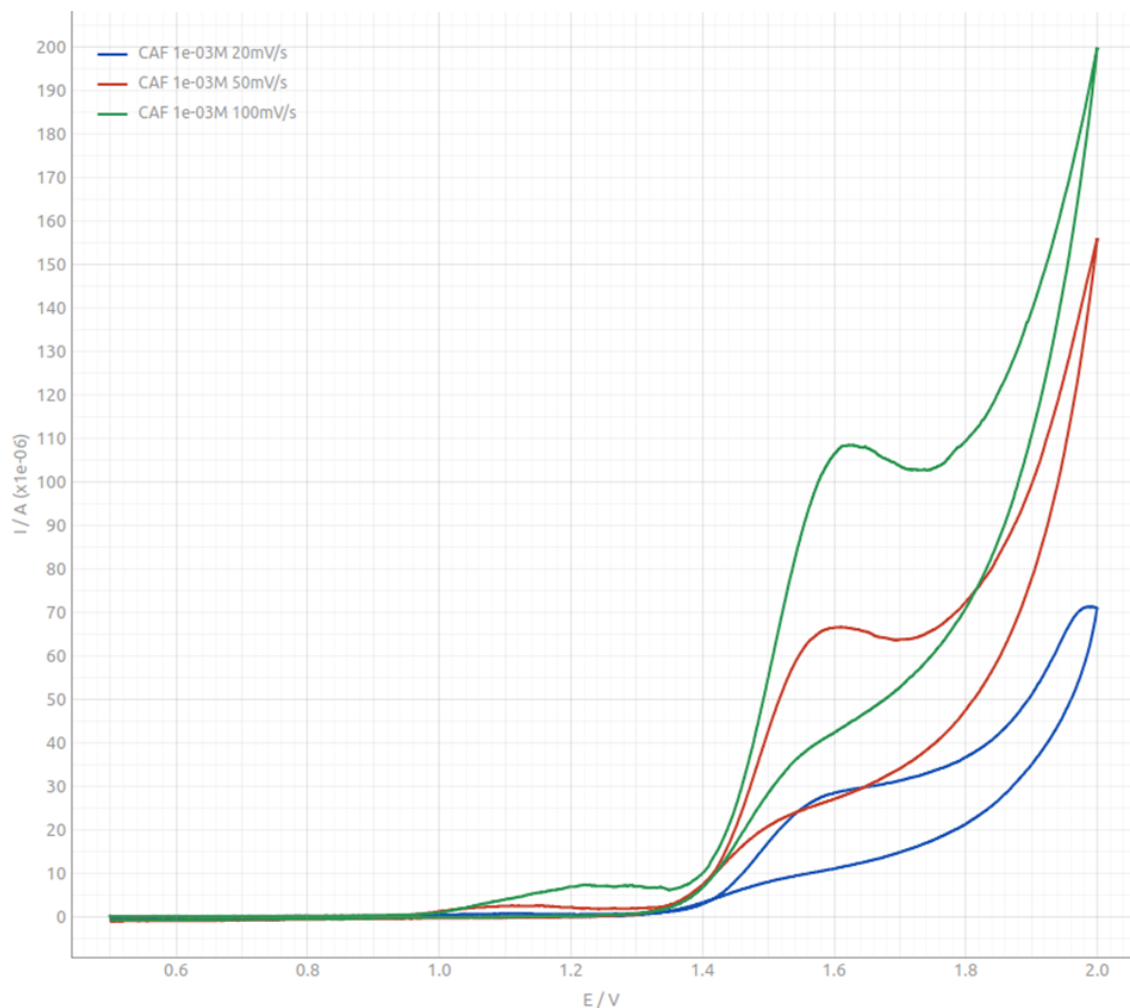


Figure 2 Cyclic voltammograms obtained for $1 \cdot 10^{-3}$ M caffeine solution in Britton–Robinson buffer using a graphite pencil electrode (PGE) at scan rates of 20, 50, and 100 mV/s

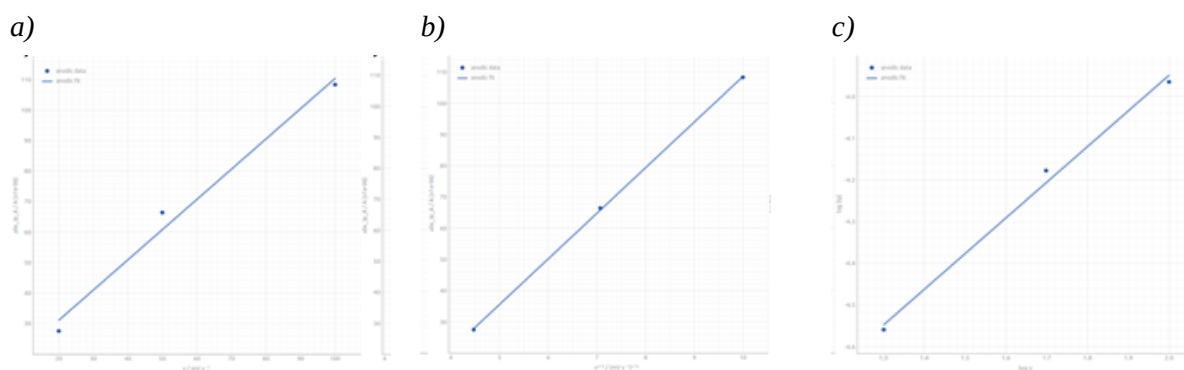


Figure 3 Regression relationships obtained for anodic peaks, current dependence on scan rate: a) I_p vs v ; b) I_p vs $v^{1/2}$; and c) $\log(I_p)$ vs $\log(v)$

Table 1 Regression parameters and anodic peaks obtained for caffeine oxidation at different scan rates using a graphite pencil electrode (PGE)

Concentration	Peak	Scan rate (mV/s)	E_p (V)	I (mA)	Regression	Slope b	Intercept	R^2	R
$1 \cdot 10^{-3}$ M	Anodic	20	1.5860	0.0275	I_p vs v	~ 0	~ 0	0.9851	0.9925
	Anodic	50	1.6002	0.0664	I_p vs $\sqrt{v}$	~ 0	~ 0	0.9998	0.9999
	Anodic	100	1.6207	0.1083	$\log(I_p)$ vs $\log(v)$	0.8566	-5.6620	0.9930	0.9965

Figure 3 presents regression relationships obtained for anodic peak current dependence on scan rate, including I_p vs v , I_p vs $\sqrt{v}$, and $\log(I_p)$ vs $\log(v)$. Table 1 summarizes the corresponding regression parameters. The obtained regression coefficients indicate a strong dependence between anodic peak current and scan rate. The I_p vs $\sqrt{v}$ relationship exhibited the highest correlation coefficient ($R^2 = 0.9998$), suggesting a significant diffusion contribution to the oxidation process of caffeine on the graphite pencil electrode surface.

The slope obtained from the $\log(I_p)$ vs $\log(v)$ regression analysis was 0.8566, indicating a mixed-controlled electrochemical process involving both diffusion and surface-related adsorption effects. Such behavior is consistent with previously reported electrochemical responses of caffeine on carbon-based electrodes and may also be influenced by the heterogeneous structure and electroactive surface variability of graphite pencil electrodes. The obtained results demonstrate that graphite pencil electrodes combined with Python-assisted electrochemical data analysis represent a suitable low-cost approach for electrochemical characterization of caffeine [5,8–11].

CONCLUSION

The obtained results demonstrate that PGEs can be successfully applied for the electrochemical characterization of caffeine in BR buffer using cyclic voltammetry. The investigated system exhibited predominantly irreversible electrochemical behavior with a clear dependence of anodic peak current and peak potential on scan rate. Regression analysis indicated a significant diffusion contribution together with surface-related effects during the oxidation process of caffeine on the graphite pencil electrode surface.

The developed Python-assisted workflow enabled systematic visualization, regression analysis, and interpretation of cyclic voltammetry data using open-source computational tools. The combination of low-cost graphite pencil electrodes and accessible Python-based data processing represents a promising approach for simple and reproducible electrochemical analysis.

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