

Short Communication

Low-cost and easy-to-use light spectroscopy can be used to monitor release behavior of essential oils

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Abstract

Patchouli oil is considered a crucial ingredient for perfume, cosmetic, food and beverage manufacturing. Evaluating the volatility behavior of patchouli oil is important because it influences the aroma profile, quality, formulation, shelf life, therapeutic efficacy, and economic value of the oil. The aim of this study was to explore the ability of a low-cost and easy-to-use light-spectral triad sensor for the assessment of evaporation behavior of patchouli oil. We used a portable SparkFun Triad Spectroscopy Sensor comprised of three sensors including AS72651 (near-infrared range), AS72652 (visible range), and AS72653 (ultra-violet range). The sensor was connected to its Arduino-compatible microcontroller (SparkFun RedBoard) through Qwiic Connect System. The sensor's onboard microcontroller facilitated the collection of spectral data across 18 channels, encompassing wavelengths from 410 nm to 940 nm. The spectral data were observed qualitatively to determine the most optimum wavelength for analyzing the evaporation behavior. The data were modeled using autoregressive integrated moving average (ARIMA). Our findings revealed that the spectral intensity is distinguishable at $\lambda=535$ nm. The ARIMA modeling indicated that the crude essential oil follows an ARIMA (0,1,0) model with drift, characterized by a negative drift parameter of -1.35 (standard error (SE): 0.33; $\sigma^2=0.74$). In contrast, the heavy fraction is best described by an ARIMA (0,0,0) model with a non-zero mean of 450.33 (SE: 0.35; $\sigma^2=0.86$). Ljung-Box test suggested the absence of significant autocorrelation for both crude ($p=0.33$) and heavy fraction patchouli oil ($p=0.5$). In conclusion, the light spectroscopy is potential for monitoring the evaporation behavior of patchouli oil, though optimization remains necessary.

Keywords: Essential oil, patchouli oil, quality control, sensor, spectroscopy

Introduction

Essential oils are concentrated hydrophobic liquids comprising volatile aroma compounds from plants. They have been widely used in various industries, including perfumery, cosmetics, food and beverages, and aromatherapy [1-3]. The popularity of these substances is largely due to their unique aromatic profiles and purported therapeutic benefits, such as antimicrobial, anti-inflammatory, and mood-enhancing effects [4,5]. Essential oils contain a diverse range of bioactive compounds which include terpenes, alcohols, esters, and aldehydes, which contribute to their broad spectrum of health benefits. For example, essential oils exhibit antioxidant properties that help in neutralizing free radicals, reducing oxidative stress, and potentially



lowering the risk of chronic diseases [6,7]. Patchouli oil, in particular, is renowned for its rich, musky-sweet fragrance and therapeutic properties (such as antidepressant, anti-inflammatory, and antimicrobial effects) [8,9].

Understanding the release or evaporation behavior of essential oils is crucial for optimizing their use in various applications [8]. This behavior influences the aroma profile, efficacy, stability, and shelf life of essential oil products. In the context of drug release and exposure, evaporation behavior is a key factor in determining the rate and extent of active compound delivery [10,11]. For instance, in topical formulations, the evaporation of essential oils can modulate the release of therapeutic agents, affecting their penetration through the skin and subsequent bioavailability [12]. Similarly, in aromatherapy, the rate of evaporation dictates the intensity and duration of exposure to aromatic compounds, influencing therapeutic outcomes. Despite the importance of monitoring evaporation, many traditional methods are expensive, complex, and not easily accessible, hindering their widespread application in research and industry [13,14].

Recent development in sensor technology have introduced affordable and user-friendly solutions that could revolutionize the way evaporation behavior is monitored. Light spectroscopy, in particular, offers a non-invasive method for analyzing essential oils by measuring their interaction with different wavelengths of light [15]. This technique can potentially assess the volatility and evaporation dynamics of essential oils, providing valuable insights into their chemical composition and behavior over time. In a previous study, the sensor has been used to capture gases released from coffee beans [16] and landfill soils [17]. The novelty of this study lies in the application of the SparkFun Triad Spectroscopy Sensor for the analysis of essential oil evaporation, specifically focusing on the evaporation behavior of crude and heavy fraction patchouli oils. This research aims to establish a new low-cost method for monitoring essential oil release. Further, we perform a direct comparison of the evaporation profiles of different oil fractions.

Methods

Materials and equipment

This study utilized crude patchouli oil and heavy fraction patchouli oil. The extraction and fractionation of patchouli oil had been reported in a previous report [9]. These samples were procured from Atsiri Research Center (Universitas Syiah Kuala, Banda Aceh, Indonesia) and stored in a dark and sealed bottle at room temperature ($25\pm 1^\circ\text{C}$).

A SparkFun Triad Spectroscopy Sensor was employed as the light spectrometer equipped with three light-emitting diodes, namely AS72651 (near-infrared range), AS72652 (visible range), and AS72653 (ultra-violet range). The sensor was connected to a SparkFun RedBoard via the Qwiic Connect System for data acquisition.

Experimental setup and data acquisition

The patchouli oil was drop-wised onto a cellulosic paper (size: 2 cm × 10 cm) until it evenly covered the area. The paper was placed on a flat surface, and a SparkFun Triad Spectroscopy Sensor AS7265x (SparkFun Electronics, Colorado, the United States) was positioned beside the sample at a fixed distance of 5 cm, perpendicular (90°) to the sample. On the opposite side of the sensor, a white cardboard was positioned at a 90° angle to as a reflective background. Before the start of each experiment, the sensor system was calibrated using a blank sample to account for ambient light conditions. Once the sample was placed, the sensor was immediately activated, and data collection began. The sensor was connected to an Arduino microcontroller, which was linked to a laptop via a USB cable, allowing spectral data to be recorded in real-time using the "Data Streamer" add-in in Microsoft Excel. Data acquisition continued for a duration of 10 minutes, capturing the spectral intensity changes at intervals of 1 second. The entire experimental setup, including the sensor alignment and sample placement, was housed in a controlled environment with ambient temperature maintained at $25\pm 1^\circ\text{C}$ and relative humidity at $50\pm 5\%$. The schematic diagram illustrating the equipment set-up during the data acquisition is presented in **Figure 1**.

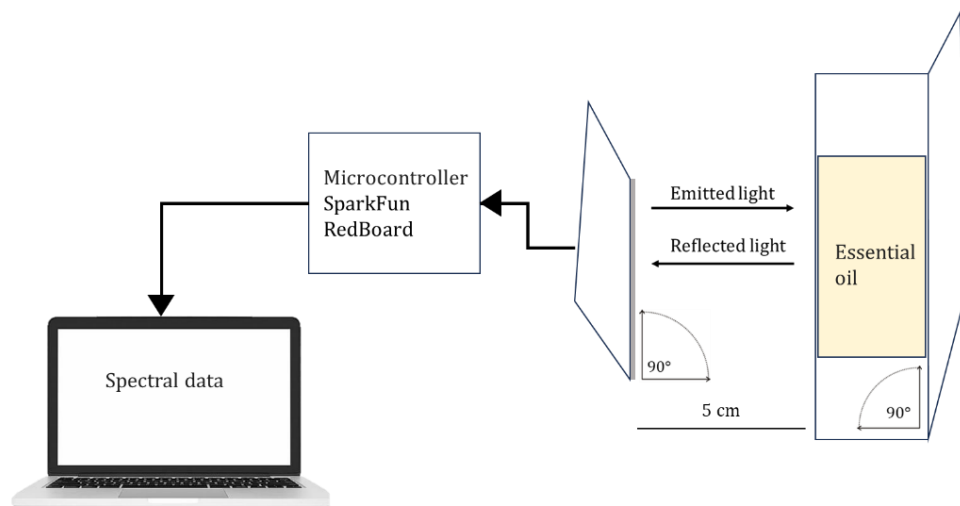


Figure 1. Schematic diagram of the sensor set-up to detect the released essential oil from the cellulosic paper.

Data analysis and modeling

The preprocessed data were imported into RStudio version 2024.04.2 for autoregressive integrated moving average (ARIMA) modeling. The `auto.arima` function from the `forecast` package was utilized to determine the most suitable ARIMA model for each oil sample, based on Akaike Information Criterion (AIC). Residuals from the fitted models were analyzed for autocorrelation using the Ljung-Box test, confirming the adequacy of the models. The residuals were further examined for normality and randomness to validate model assumptions. Model performance was evaluated using various error measures, including mean absolute error (MAE), root mean square error (RMSE), and mean absolute percentage error (MAPE).

Results

Spectral profile

Distinct spectral profiles for crude and heavy fraction patchouli oils were observed at the wavelength of $\lambda=535$ nm, which was determined to be the most optimal for monitoring evaporation behavior (**Figure 2A** and **2B**). The spectral intensity for crude patchouli oil ranged from 423.91 ± 0.7 to 417.14 ± 0.4 a.u., with decreasing trend in intensity over time (**Figure 2C**). The spectral intensity for the heavy fraction patchouli oil was observed to be relatively stable, ranging from 450.97 ± 0.4 to 448.86 ± 0.4 a.u. (**Figure 2D**).

Evaporation behavior based on ARIMA

The evaporation behavior of crude and heavy fraction patchouli oils was assessed using ARIMA modeling of spectral intensity data, where the plots are presented in **Figure 3**. For the crude patchouli oil, the ARIMA (0,1,0) model with drift revealed a steady decrease in intensity over time. The forecasted trend predicted a continued decline in intensity, with the 95% CIs reflecting increasing uncertainty over time. In contrast, the heavy fraction patchouli oil, modeled using ARIMA (0,0,0) with a non-zero mean, exhibited a stable intensity profile with minimal fluctuations. No significant autocorrelation was observed in the autocorrelation function (ACF) plots for the residuals of both models (**Figure 3C** and **3D**).

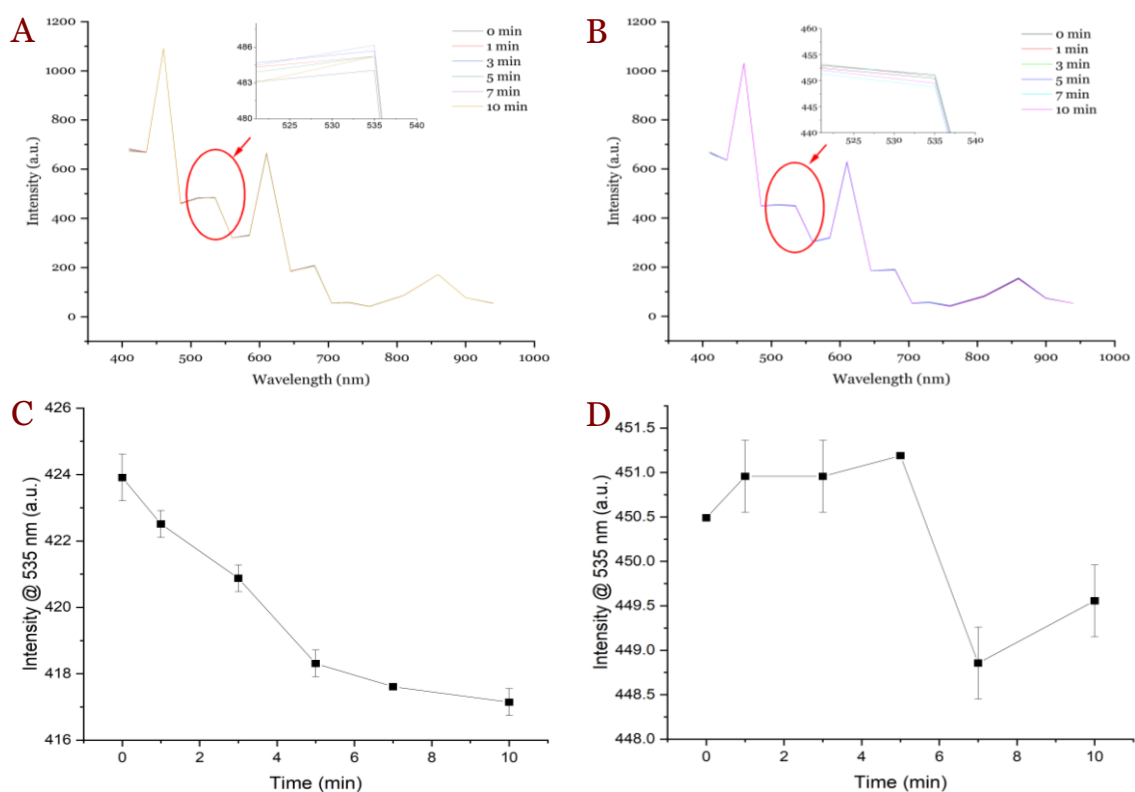


Figure 2. Spectral profile of crude fraction (A) and heavy fraction (B) of patchouli oil. Spectral intensity at 535 nm for crude fraction (C) and heavy fraction (D) of patchouli oil.

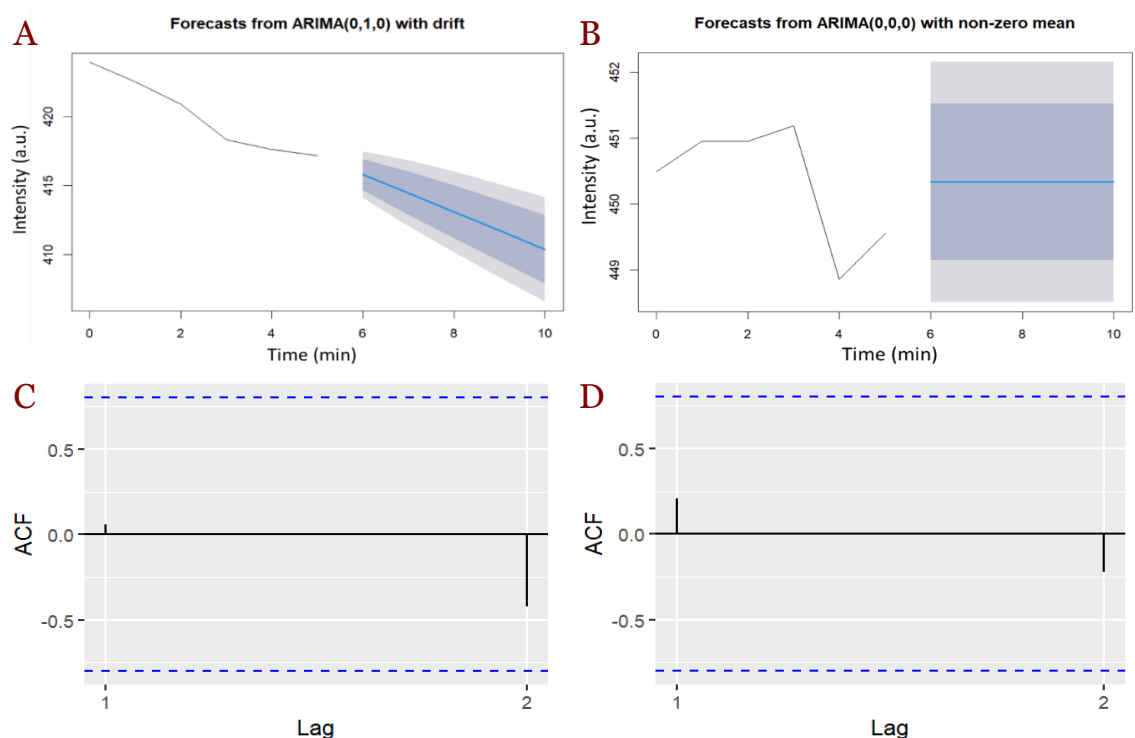


Figure 3. Forecast and residual analysis of spectral intensity data for crude and heavy fraction patchouli oils using ARIMA models. Forecast from ARIMA (0,1,0) with drift for crude patchouli oil, showing a steady decline in intensity with the forecasted trend and 95% CIs (A). Forecast from ARIMA (0,0,0) with non-zero mean for heavy fraction patchouli oil, indicating stable intensity with no significant trend (B). Autocorrelation function (ACF) plots for the residuals of crude (C) and heavy fraction oils (D), respectively, showing no significant autocorrelation, indicating that the ARIMA models adequately captured the data trends.

Discussion

The analysis of the release characteristics of crude essential oil and its heavy fraction provides valuable insights into their chemical composition and potential applications. Using ARIMA modeling, the crude essential oil exhibited a linear decrease in mean intensity over time, best captured by the ARIMA (0,1,0) model with drift. This model's negative drift parameter indicates a uniform rate of evaporation, suggesting a steady and predictable loss of volatile components. According to a previous study, the crude fraction of patchouli oil contains α -guaiene, α -patchoulene, β -patchoulene, globulol, caryophyllene, and trans-longipinocarveol [9], which could collectively contribute to the steady release behavior. These terpenes and sesquiterpenes are known for their high volatility, which results in a continuous evaporation process [18]. In the present study, the model's residuals resembling white noise imply that the primary dynamics of evaporation are effectively captured. The uniform evaporation rate makes crude essential oil suitable for applications requiring a consistent release of aroma or active compounds, such as in diffusers, air fresheners, or therapeutic products, where rapid diffusion is advantageous [19].

Conversely, in the present study, the heavy fraction of essential oils displays a stable evaporation profile, characterized by the ARIMA (0,0,0) model with a non-zero mean. The mean intensity remains constant over time, indicating a stable concentration. This stability is attributed to the presence of less volatile compounds like patchouli alcohol, which have a slower and more uniform evaporation rate. As reported previously, the heavy fraction lacks the more volatile components found in the crude essential oil contributing to its reduced evaporation rate [9]. This slower evaporation is advantageous for applications requiring long-lasting effects, such as perfumes, lotions, or other products where prolonged scent or active ingredient presence is desired [20]. The comparative analysis, in the present study, highlights the distinct volatility profiles between the crude essential oil and the heavy fraction, where the latter contains more volatile compounds.

While this study demonstrates the potential of the SparkFun Triad Spectroscopy Sensor for monitoring the evaporation behavior of patchouli oil, several limitations should be acknowledged. The controlled experimental conditions may not fully capture the impact of fluctuating environmental factors such as temperature and humidity, which could influence real-world evaporation behavior. Additionally, the short observation period might not reveal the complete evaporation profile, particularly for slower-evaporating fractions. The study's findings are limited to patchouli oil, necessitating further research to validate the method across a broader range of essential oils. Moreover, the study did not compare this spectroscopy method with traditional techniques, which would be useful for validating its accuracy. Finally, the analysis was conducted on a specific substrate (cellulosic paper), and results may vary with other substrates or formulations, indicating the need for broader testing in diverse applications.

Conclusion

Our findings suggest that SparkFun Triad Spectroscopy Sensor can be used as a low-cost monitoring tool for evaporation behavior of patchouli oil. The distinctive evaporation behaviors for crude and heavy fraction samples were observed through ARIMA modeling. The crude essential oil exhibited a steady evaporation trend, captured by an ARIMA (0,1,0) model with drift, indicative of its higher volatility. In contrast, the heavy fraction, characterized by an ARIMA (0,0,0) model with a non-zero mean, reflecting its lower volatility. In future studies, the utility of this sensor can be optimized by considering the effects of ambient temperature, humidity, and airflow. Additionally, the potential to monitor essential oil release from a specific product formulation can be investigated.

Ethics approval

Not required.

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Competing interests

The authors have no known conflict of interest in relation to the publication of this work.

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Underlying data

Data underlying this study can be requested from the corresponding authors upon reasonable request.

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