

Research Article

Kinetic evaluation of the microwave-assisted hydrodistillation process for 2-phenylthiolane extraction from jasmine flowers

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ABSTRACT

Microwave-assisted hydrodistillation (MAHD) presents an effective substitute to traditional extraction techniques in the isolation of bioactive compounds from plant materials. However, limited kinetic data exist on the extraction behavior of 2-phenylthiolane from jasmine flowers using MAHD, and the underlying mass-transfer mechanisms remain insufficiently explored. This work investigates the kinetic models of 2-phenylthiolane extraction from jasmine blossoms using MAHD under varying conditions of time, microwave power levels, and solid-to-liquid ratios. Among the models examined, the second-order kinetic model had the highest accuracy ($R^2 = 0.976$), outperforming the first-order model and providing the best description of the two distinct extraction stages the rapid washing phase and the slower diffusion phase. Optimal extraction conditions were observed at 400 W microwave power and a solid-to-liquid ratio of 1.5 g/20 mL. The findings from this study show that following the second-order kinetic model, 2-phenylthiolane extraction can be precisely regulated, scaled up for industrial production, and the product quality and yield can be monitored and controlled for pharmaceutical applications. The study also contributes to advancing economical and environmentally friendly production techniques. All things considered, this model provides a strong basis for developing bioactive component extraction via MAHD, stimulating green technology innovation, and improving the economic feasibility of natural product recovery.

1. Background

Essential oils are volatile aromatic compounds extensively utilized across various industries (Rassem *et al.*, 2018). They are complex mixtures comprising hydrocarbons, phenols, alcohols, ketones, aldehydes, and esters (Rassem *et al.*, 2018). These oils, extracted from a wide range of plants, are commercially available for various applications (Bolouri *et al.*, 2022). Notably, research has demonstrated that even minimal quantities of essential oils can exert significant effects on biological activities (Oussalah *et al.*, 2006; Oussalah *et al.*, 2007).

The Jasmine plant, native to tropical regions such as Africa, Australia, and Southeast Asia, is now cultivated extensively across the globe. In Malaysia, the plants flourish year-round without seasonal disruptions because they grow in a steady tropical climate, where temperatures rarely fall below 10°C. This study examines the essential oils extracted from Malaysian Jasmine flowers, focusing on the Melati and Melur varieties. Renowned for providing the characteristic fragrance and flavor associated with Jasmine, these essential oils owe their biological and physicochemical properties to their distinctive terpene, terpenoid,

and hydrocarbon compositions. Traditionally, Jasmine essential oils have been utilized as expectorants, treatments for dry skin, and agents with antiseptic, antispasmodic, and antidepressant properties. They are also used to manage conditions including depression, fatigue, sensitive skin, migraines, and respiratory ailments. Moreover, Jasmine flowers are rich in a range of bioactive compounds such as fatty acids, flavonoids, carbohydrates, proteins, and minerals (Jha *et al.*, 2022). Many studies have examined its many health-promoting qualities, emphasizing their cytotoxic, antibacterial, antioxidant, anti-inflammatory, antihypertensive, hepatoprotective, anticancer, antidiabetic, and antinociceptive effects (Higginbotham *et al.*, 2014).

2-Phenylthiolane, the predominant bioactive compound found in jasmine flowers (Rassem *et al.*, 2018), is renowned for its diverse biological activities, including antioxidant, antiviral, antibacterial, antihypertensive, anti-inflammatory, antithrombotic, cytotoxic, and anticancer effects (Rassem *et al.*, 2017; Higginbotham *et al.*, 2014). It is a promising scaffold for the creation of new medicinal compounds because of its complex functional groups. Depending on the plant source

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and the particular chemicals targeted, extraction procedures can be customized to separate valuable compounds from botanical materials.

In the past, traditional methods such as steam distillation (Dao et al., 2021) and hydrodistillation (Dao et al., 2020) were used to extract essential oils and medicinal compounds from plants. However, developments have given rise to contemporary methods, including solvent-free and microwave-assisted extraction (Dao et al., 2021). Although classical methods are still widely used because of their ease and efficiency in processing aromatic plants, they have drawbacks such as high energy and solvent requirements, poor extraction efficiency, deterioration of sensitive chemicals, and lengthy operating durations (Dao et al., 2019; Dao et al., 2021).

Innovative technologies, including supercritical fluid extraction and microwave-assisted hydrodistillation (MAHD), have been developed in response to these limitations. Through the optimization of crucial parameters such as extraction temperature, time, and material-to-solvent ratio, studies have demonstrated the advantage of MAHD in recovering a broader range of bioactive compounds (Dao et al., 2019; Mandal et al., 2007). Furthermore, by increasing yields, improving product quality, and reducing energy consumption and processing costs, the incorporation of optimization tools such as response surface methodology (RSM) has improved process performance (Dao et al., 2021). These modern methods closely adhere to the concepts of sustainable manufacturing and green chemistry while significantly improving extraction results.

Reliable kinetic modeling is essential for understanding extraction mechanisms and optimizing extraction processes, as it enables prediction of extraction yields, critical evaluation of experimental data, and improvement of process efficiency (Variyana and Mahfud, 2020). However, the kinetic behavior of 2-phenylthiolane extraction from jasmine flowers remains largely unknown (Dao et al., 2022). The effects of extraction time, microwave power, and liquid-to-solid ratio during MAHD are therefore systematically investigated in this study using first- and second-order kinetic models. The study aims to evaluate the suitability of these models for describing the mass-transfer behavior of 2-phenylthiolane under microwave-assisted conditions. Compared with conventional hydrodistillation, MAHD is expected to offer faster and more energy-efficient extraction with reduced operational costs. Furthermore, the combined application of the Peleg and Hervás kinetic models is explored as a predictive framework for characterizing extraction kinetics. Overall, this work seeks to establish a systematic kinetic basis for 2-phenylthiolane extraction from jasmine flowers and to provide insights relevant to process optimization and industrial application, being the first systematic kinetic modeling of 2-phenylthiolane extraction (Phat et al., 2020).

2. Materials

Blemish-free jasmine flowers (without physical impurities, microbiological contamination, or insect infestation) were harvested from Kuantan, Pahang, Malaysia (3.8167° N, 103.3333° E). The harvested sample was extensively cleaned by rinsing with distilled water for 30 minutes to remove all surface impurities, such as sand. The fresh jasmine flowers were then dried for two days at 45 - 55 °C, pulverized, and sieved using a mechanical sieve shaker to obtain 80 µg particle size jasmine powder. To ensure environmental safety and experimental consistency, only analytical-grade solvents and chemicals (≥ 99% purity) supplied by Sigma-Aldrich were used in the oil extraction process, including methanol, dimethyl sulfoxide, sodium acetate, and 2-hydroxy-1,7-dimethoxyxanthone.

3. Methods

3.1 Microwave-assisted hydrodistillation

For MAHD, 70 g of dried jasmine flower powder was extracted using 1000 mL of 95% methanol in a condenser-equipped Ethos microwave extractor (2450 MHz, Milestone, Italy) (Rassem et al., 2018). The vessels were allowed to cool to room temperature before opening, and the extraction parameters were systematically varied as follows: solid-to-liquid ratio (0.50–3.0 g/20 mL), extraction time (20–160 seconds

at 20-second intervals), and microwave power (200–1200 W). The extracts were diluted in dimethyl sulfoxide after solvent evaporation, and analyzed using a UV-Vis spectrophotometer (Spectroquant® Pharo 100 M). Tests were conducted in triplicate for each condition.

3.2 Determination of total 2-phenylthiolane content via colorimetric analysis

The colorimetric technique, supported by visible light spectroscopy, is commonly employed to analyze complex natural product mixtures (Dai, 1999). In this study, it was used to quantify 2-phenylthiolane in jasmine flower extracts. The process creates a yellow complex that absorbs at 450 nm by oxidizing 2-phenylthiolane with 10% sodium acetate (Negi et al., 2013). 100 µL of the microwave-extracted sample was mixed with 40 µL of sodium acetate, and the mixture was left for 60 minutes at room temperature. The absorbance was measured at 450 nm using a UV-Vis spectrophotometer. Standard solutions of 2-hydroxy-1,7-dimethoxyxanthone were used to prepare a calibration curve with concentrations ranging from 0 to 0.20 µL in increments of 0.04 µL. The concentration of 2-phenylthiolane was calculated and represented as equivalents per gram of dry extract (2-PhT/gP).

3.3 Kinetic modeling of the extraction process

The extraction kinetics were evaluated using first- and second-order kinetic models. These models helped determine extraction rates and gave better understanding of the solute-solvent interactions and diffusion processes. Applying both models offered key insights into the mechanisms governing 2-phenylthiolane release, supporting the optimization of extraction conditions and improving process efficiency.

3.3.1 The model proposed by hervas et al.

Eq. (1) presents the kinetic mechanism described in the Hervás model (Hervás et al., 2006), which was used to examine the extraction process at equilibrium.

$$\frac{dC}{dt} = K(C_0 - C) \quad (1)$$

Here, K is the effective diffusion coefficient (µL/µg 2-PhT/s), C_0 is the initial concentration 2-phenylthiolane (µg 2-PhT/mL), and C is the concentration 2-phenylthiolane (µg 2-PhT/mL) at any given time t .

The relevant boundary constraints $C|_{t=0} = 0$ and $C|_{t=t} = C_t$ are included in Eq. (2), which is obtained by integrating Eq. (1) from the initial time to a particular time t .

$$C(t) = C_0 * (1 - e^{-kt}) \quad (2)$$

3.3.2 The peleg model

The following equation illustrates how the extraction process was described using a modified version of the Peleg model (Peleg, 1988) as represented in Eq. (3):

$$C(t) = \frac{t}{K_1 + K_2 * t} \quad (3)$$

In this model, t is the extraction time in seconds, and C_t is the concentration of 2-phenylthiolane at time t (given in µg 2-PhT/g). Peleg's rate constant (s•g/µg 2-PhT) is denoted by K_1 , and its capacity constant (g/µg 2-PhT) by K_2 .

The initial extraction rate (B_0) at the beginning of the process, or when ($t = t_0$), is represented by the Peleg rate constant K_1 in Eq. (4)

$$B_0 = \frac{1}{K_1} \quad (4)$$

The maximum extraction yield, which represents the equilibrium concentration of 2-Phenylthiolane (C_e) as time approaches infinity ($t \rightarrow \infty$), is associated with the Peleg capacity constant K_2 . The connection between the equilibrium concentration and the K_2 constant is seen in Eq. (5).

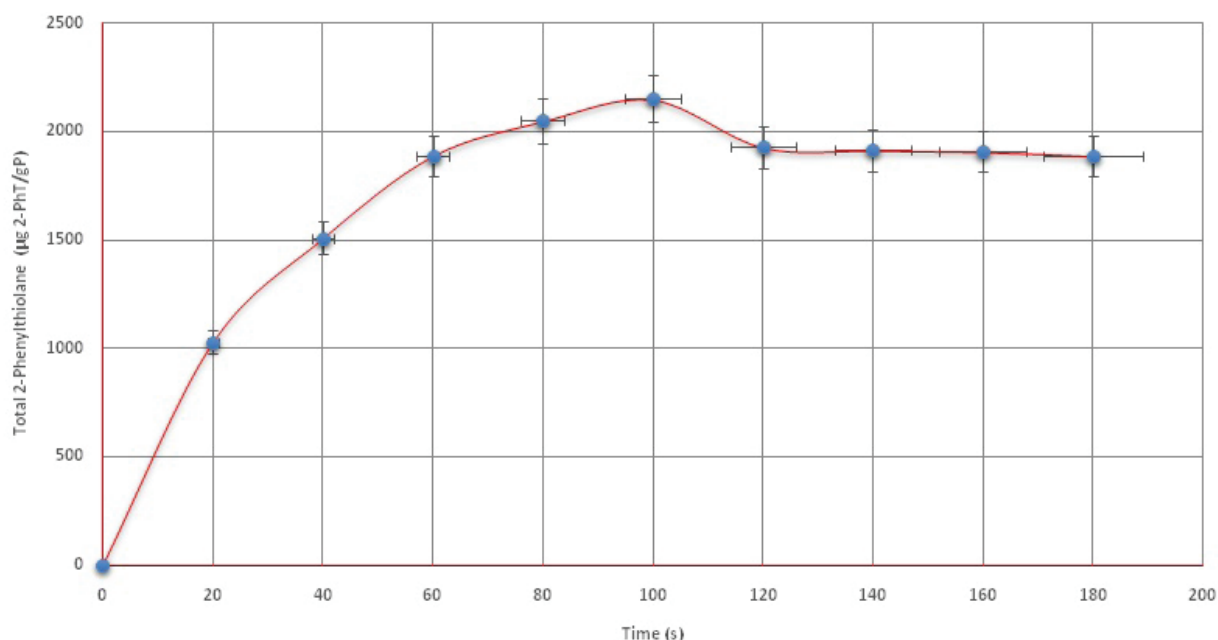


Fig. 1. Shows how the length of extraction affects the 2-phenylthiolane concentration during microwave-assisted hydrodistillation.

$$C_0 = \frac{1}{K_2} \quad (5)$$

As a result, the extraction rate constant is expressed according to Eq. (6).

$$K = \frac{K_2}{K_1} \quad (6)$$

3.3.3 The gaussian-based model

A Gaussian model was used to simulate the extraction process, with modifications made to suit the specific conditions as represented in Eq. (7):

$$Y = a * \exp \left[-0.5 * \left(\frac{(x - x_0)}{k} \right)^2 \right] \quad (7)$$

In this model, x is an independent variable in the extraction process, X_0 is the precise value of X at which the maximum extraction rate occurs, K is a constant associated with the extraction rate, Y is the extraction rate, and a is the highest extraction rate that can be achieved.

3.4 Data analysis and statistical evaluation

The results are presented as mean values with standard errors, and each experiment was carried out in triplicate to ensure accuracy and minimize variability between trials. One-way ANOVA (Analysis of Variance) was used to assess statistical significance, with a P-value < 0.05 considered significant, indicating that differences between groups are statistically meaningful if the P-value is below this threshold. The Statgraphics Centurion XII program was used to conduct the analysis, providing comprehensive statistical tools for data evaluation, visualization, and multi-variable analysis.

4. Results

4.1 Influence of extraction time on the yield of 2-phenylthiolane

Fig. 1 shows the clear three-stage behavior of the extraction kinetics of 2-phenylthiolane from jasmine flowers using MAHD. The rapid rise

in 2-phenylthiolane concentration over the first 60 seconds indicated the fast release of easily accessible surface compounds. The extraction rate became more gradual between 60 and 100 seconds, indicating a shift to a diffusion-controlled stage, which is controlled by internal mass transfer in the plant matrix, and the extraction rate drastically reduced between 100 and 120 seconds. The concentration started to converge toward equilibrium after 120 seconds, indicating that the system was almost saturated. The Peleg and Hervas' kinetic models were used to analyze and characterize this extraction pattern.

4.1.1 The hervas model

Table 1 displays the correlation coefficient (R^2), the calculated constants K and C_0 , and the extraction kinetics data for the solid-liquid extraction using the Hervas method.

4.1.2 Peleg model

The extraction kinetics were examined in greater detail using the Peleg model. A thorough overview of the extraction parameters is provided in Table 2, which also includes the model coefficients (K_p , K_2 , and B_0), correlation coefficient (R^2), and rate constants. The trend in Fig. 2 indicates that this model accurately represents the extraction kinetics under MAHD conditions.

4.2 Influence of microwave power on the extraction efficiency of 2-phenylthiolane

The effect of microwave power on the yield of 2-phenylthiolane is illustrated in Fig. 3. Significant increase in 2-phenylthiolane

Table 1.
Hervas model for 2-phenylthiolane extraction using microwave-assisted hydrodistillation.

C_0 (µg 2-PhT/mL)	K (µg 2-PhT/mL. s)	R^2
1994.79	0.0396	0.9748

Table 2.
Peleg model for 2-phenylthiolane hydrodistillation with microwave assistance.

C_0 (µg 2-PhT/mL)	K_1 (sg/µg 2-Ph)	K_2 (µg 2-PhT/mL. s)	B_0 (µg 2-PhT/g)	R^2
1134.23	0.000429	0.000882	2329.93	0.976

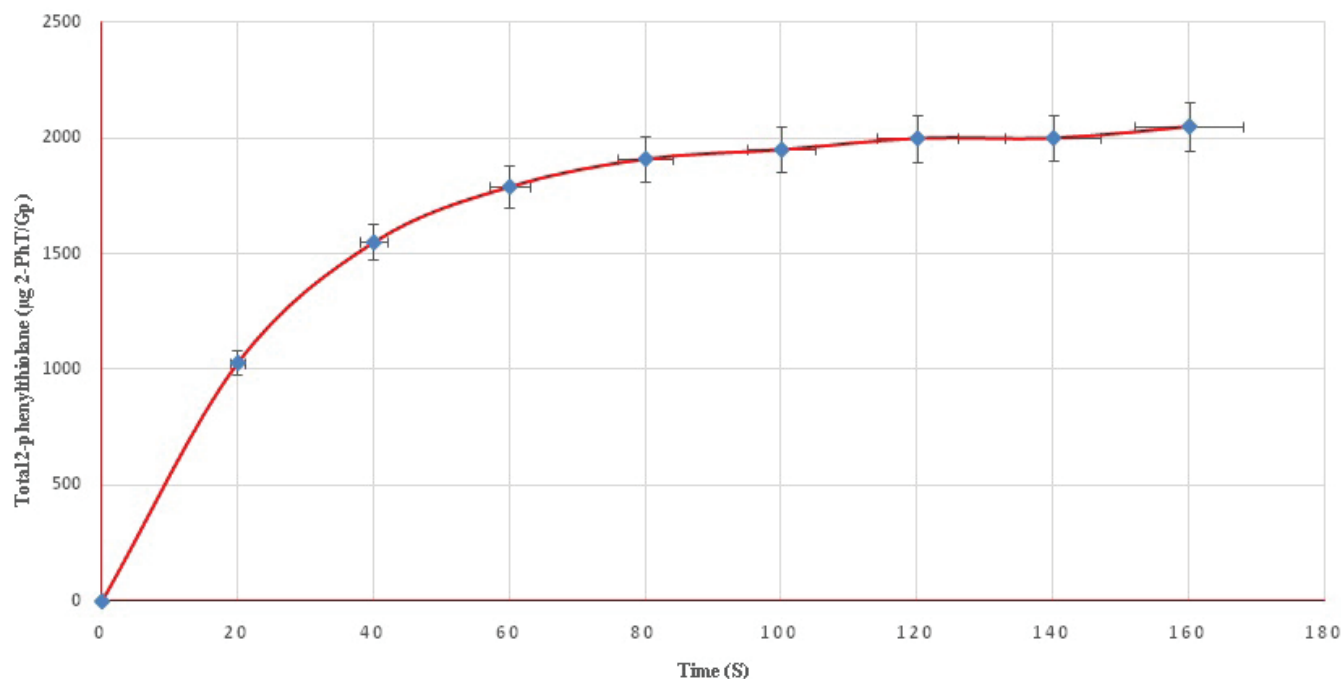


Fig. 2. The Peleg model's applicability to the kinetic investigation of 2-phenylthiolane hydrodistillation from jasmine flowers with microwave assistance.

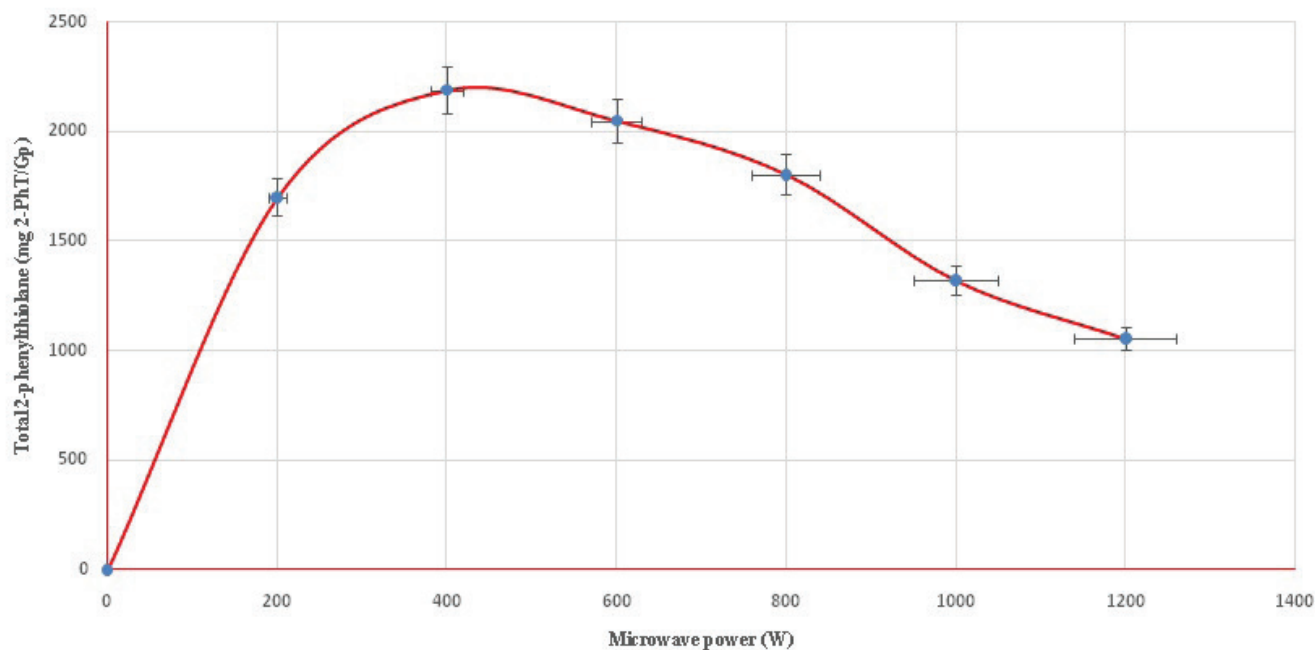


Fig. 3. Shows how microwave power affects 2-phenylthiolane concentration during extraction using microwave-assisted hydrodistillation.

concentration was observed as microwave power increased from 200 W to 400 W, after which the yield stabilized. However, at 600 W, a noticeable decline in compound concentration was detected, likely due to thermal degradation. Specifically, the concentrations of 2-phenylthiolane at 200 W and 400 W were 1702.54 µg 2-PhT/gP and 2190.21 µg 2-PhT/gP, respectively, indicating that 400 W may represent the optimal power level for maximizing extraction efficiency without compromising compound integrity.

4.3 Effect of solid-to-liquid ratio on the yield of 2-phenylthiolane extraction

Fig. 4 illustrates how the concentration of 2-phenylthiolane during MAHD is influenced by the solid-to-liquid ratio. The concentration

of 2-phenylthiolane increased gradually as the solid-to-liquid ratio increases from 0.50 to 1.5 g/20 mL. However, beyond this point, a noticeable decline in both the yield and concentration of 2-phenylthiolane occurs, indicating an optimal solid-to-liquid ratio of 1.5 g/20 mL, beyond which further increases may hinder extraction efficiency.

4.3.1 Gaussian model analysis

The microwave power and solid-to-liquid ratio data were analyzed using a Gaussian extraction model. Table 3 presents the calculated maximum extraction rate, A, model coefficients (X_0 and K), and the coefficient of determination (R^2) for the extraction process.

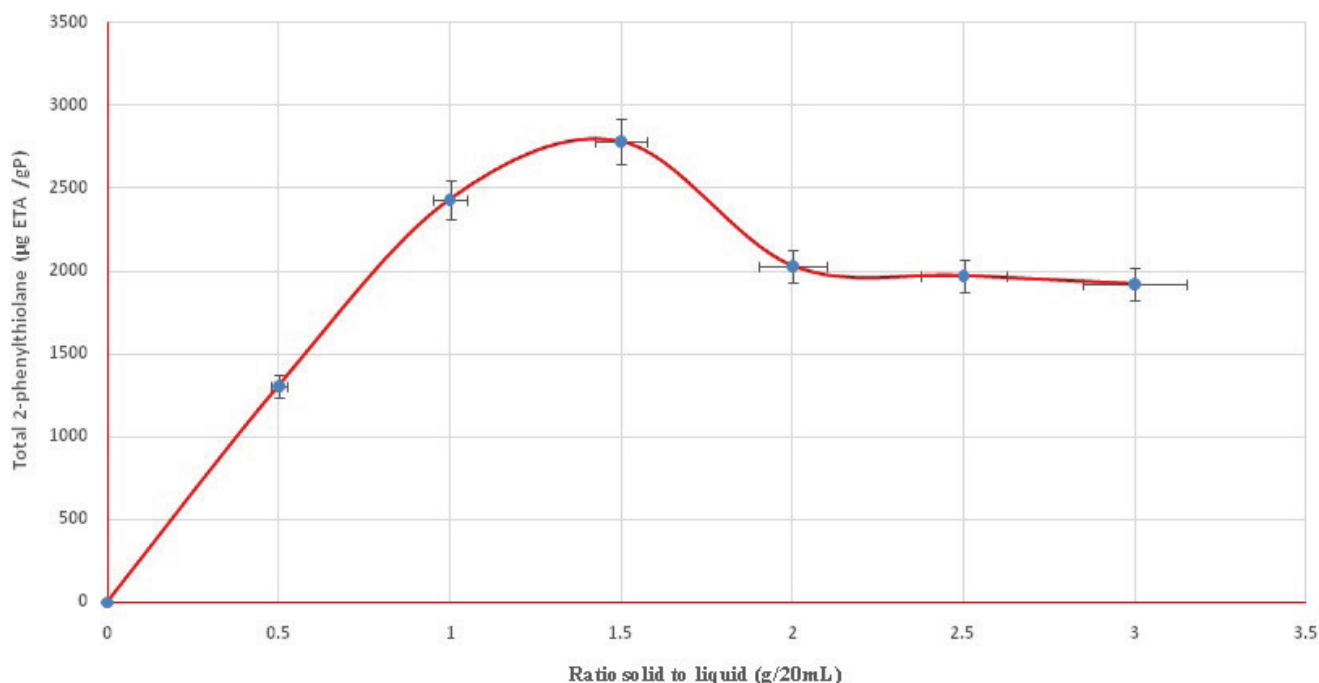


Fig. 4. Shows how the solid-to-liquid ratio affects the concentration of 2-phenylthiolane in the extraction process of microwave-assisted hydrodistillation.

Table 3.

Gaussian model parameters for the microwave-assisted hydrodistillation of 2-phenylthiolane.

Coefficient	Effect of microwave power	Effect of solid-liquid ratio
A	2265.85 (μg 2-PhT/gP)	2605.82 (μg 2-PhT/gP)
K	395.65 (W)	1.10 (g/20ml)
X_0	618.20 (W)	1.82 (g/20ml)
R^2	0.765	0.735

5. Discussion

5.1 Impact of extraction time on the yield of 2-phenylthiolane extraction

This study offers a kinetic evaluation of the recovery of 2-phenylthiolane from jasmine flowers by MAHD. The concentration profile of 2-phenylthiolane over time is shown in Fig. 1. The quick extraction phase is initially identified by a sharp rise in 2-phenylthiolane concentration during the first 60 seconds. The concentration then rises more gradually over the next 40 seconds, approaching equilibrium as the procedure comes to a close. This trend indicates that there was a rapid release of readily extractable compounds from the plant particles' surface, followed by a delayed diffusion of less soluble components. 2-Phenylthiolane's concentration-time curve resembles moisture sorption curves, indicating that comparable mass transfer models could be used to explain both processes. Peleg's and Hervás mathematical models were used for the extraction kinetics.

5.1.1 Hervás model

Table 1 presents the kinetic parameters of the extraction process using the Hervás model. Even though the first extraction stage shows partial conformance, the poor correlation coefficients show that the total extraction behavior does not fit well within a first-order kinetic framework. To gain a deeper understanding of the process, the Peleg model was also applied. This model yielded extraction constants, a higher coefficient of determination (R^2), and specific parameters K_1 , K_2 , and k , as detailed in Table 2. The improved fit of the Peleg model highlights its superior ability to describe the dynamics of the MAHD process. In contrast, Gotama et al. (2023) applied the Power

Law model without clearly explaining the extraction mechanism. The better fit obtained in the present study indicates that the extraction of 2-phenylthiolane under MAHD follows a more complex two-phase pathway, involving an initial washing stage followed by a diffusion-controlled stage.

In the case of 2-phenylthiolane extraction, the MAHD process begins with a rapid solubilization of easily accessible compounds. This is followed by a secondary phase marked by a slower release of soluble molecules, likely due to structural resistance within the plant matrix and limited internal diffusion. This latter phase, governed by external diffusion and changes in the physical integrity of the material, significantly affects the overall extraction kinetics, as also discussed in (Kusuma and Mahfud, 2017).

5.2 Effect of microwave power on the extraction yield of 2-phenylthiolane

Fig. 3 shows how the concentration of 2-phenylthiolane during the extraction process is affected by microwave power. As microwave power increases from 200 to 400 W, the findings show a progressive increase in compound yield, with concentrations of 1702.54 μg 2-PhT/gP and 2190.21 μg 2-PhT/gP, respectively. The yield reaches a peak around 400 W and then noticeably drops at 600 W. The impact of microwave energy on molecular interactions through ionic conduction and dipole rotation is believed to be responsible for this initial increase in extraction efficiency. Both the plant matrix and the solvent are rapidly heated volumetrically as a result of these processes, increasing the solubility and release of target chemicals by promoting molecular mobility, enhancing solvent penetration, softening plant tissues, and upsetting cellular structures (Tsatsop Tsague et al., 2020).

The observed reduction in 2-phenylthiolane concentration at 600 W is likely due to thermal degradation of the compound under excessive microwave energy. Since the experiments were conducted using dry plant material, the decrease cannot be attributed to evaporation or drying effects (Kullu et al., 2014). This trend of an initial increase followed by a decline at higher power levels reflects similar observations reported in the MAHD extraction of astragalosides from *Radix astragali*, where excessive microwave intensity led to reduced yields due to disrupted molecular interactions and compound degradation (Yan et al., 2010).

5.3 Impact of solid-to-liquid ratio on 2-phenylthiolane extraction yield

Prior studies by Pompeu et al. and Gan and Latiff have emphasized the crucial part this ratio plays in the effectiveness of phenolic

compound extraction. According to Pompeu *et al.*, the best ratio for removing appreciable levels of phenolics from *Euterpe oleracea* fruits was 20:1 (mL/g) (Pompeu *et al.*, 2009). Similarly, Gan and Latiff showed that a liquid-to-solid ratio of 20 mL/g significantly impacted the extraction yield, but extraction temperature had little to no effect on the total phenolic content (Chee-Yuen and Latiff, 2011).

5.4 Gaussian model

A Gaussian model was used to examine how the solid-to-liquid ratio and microwave power affected the extraction process. As shown in Table 3, this method yielded important information on the peak extraction rate, the coefficient of determination (R^2), and important model parameters (X_0 and K). Known for its capacity to model symmetrical distributions, the Gaussian model effectively captured the variations in 2-phenylthiolane concentration, including both the rising and declining trends. At a solid-to-liquid ratio of 1.5 g/20 mL and a microwave power of 400 W, the maximum extraction yield was recorded. This modeling approach proves instrumental in identifying optimal operational conditions within the tested parameters, ultimately enhancing extraction efficiency.

The best-fit model, the second-order kinetic model, suggests that diffusion-controlled mass transfer, not straightforward surface washing, controls the dynamics of the MAHD process. The availability of active extraction sites and solute concentration both affect the extraction rate, according to the strong agreement between the experimental data and the second-order model. This implies that the release of 2-phenylthiolane proceeds through a gradual, concentration-dependent mechanism rather than a purely first-order decay, and that internal diffusion within the plant matrix is the rate-determining step during MAHD. In order to improve internal mass transfer efficiency, the model emphasizes the significance of optimizing microwave power and heating uniformity.

6. Conclusions

This study provides an in-depth evaluation of the kinetic behavior of 2-phenylthiolane during MAHD of jasmine flowers. This study emphasizes how important extraction time and microwave power are to raising MAHD efficiency. The extraction behavior was better described by the second-order kinetic model than by the first-order model, according to a strong correlation coefficient ($R^2 = 0.976$). The study provides a better understanding of the release dynamics of 2-Phenylthiolane under microwave treatment by identifying a two-phase pathway that consists of an initial washing stage followed by a diffusion-controlled phase. Through the use of detailed kinetic modeling on jasmine flowers, a source that has received little attention, this study closes a significant gap in the literature and validates MAHD's potential as a highly efficient, sustainable, and scalable method for extracting industrial bioactive compounds. Additionally, this study offers the first systematic kinetic modeling of 2-phenylthiolane extraction using MAHD, exhibiting quick, economical, and energy-efficient performance with trustworthy predictive accuracy. Based on the experimental findings, the optimal extraction yield was achieved at a microwave power of 400 W and a solid-to-liquid ratio of 1.5 g/20 mL, indicating these as the most effective operating conditions for MAHD. Nevertheless, the results are still restricted to laboratory settings, and future research should look at broader operational factors.

CRedit authorship contribution statement

Najat Masood: Writing – review & editing, supervision, validation, conceptualization. **Hesham Hussein Rassem:** Writing – original draft, investigation, data curation, formal analysis, conceptualization, funding acquisition. **Sami M. Magam:** Writing – review & editing, methodology, formal analysis, investigation. **Anbia Adam:** Writing – review & editing, supervision, validation, conceptualization. **Gehad M. Subaiea:** Writing – review & editing, visualization, resources, data curation. **Tahani Y. A. Alanazi:** Writing – review & editing, software, investigation, data interpretation. **Esam Omar Al-Wesabi:**

Writing – review & editing, resources, project administration. **Aljazi A. AlRashidi:** Writing – review & editing, supervision, methodology, conceptualization.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper..

Data availability

The data supporting the main findings of the study are contained within the manuscript. Additional data are available from the corresponding author upon reasonable request.

Declaration of generative AI and AI-assisted technologies in the writing process

The authors confirm that there was no use of artificial intelligence (AI)-assisted technology for assisting in the writing or editing of the manuscript and no images were manipulated using AI.

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