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Solubility Modeling of Sabah Green Robusta Coffee (*Coffea canephora*) Bean Oil Extracted Using Supercritical Carbon Dioxide

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Abstract

This study investigates the solubility correlation of oil extracted from Sabah green Robusta coffee (*Coffea canephora*) beans through supercritical carbon dioxide (SC-CO_2) extraction. Sabah, recognized as the largest coffee-producing region in Malaysia, serves as a significant source of Robusta beans for this research. The solubility of coffee bean oil was evaluated under varying pressures (10–30 MPa) and temperatures (40–80 °C). The maximum solubility, 2.681 mg/g CO_2, was recorded at 30 MPa and 40 °C, whereas the lowest solubility, approximately 0.440 mg/g CO_2, occurred at 20 MPa and 80 °C. A clear inverse relationship between solubility and temperature was observed, with solubility decreasing as temperature increased to 80 °C. Conversely, elevated pressure, particularly at 30 MPa, enhanced solubility due to the increased density and solvent power of SC-CO_2. Experimental data exhibited strong agreement with Chrastil's equation, yielding a relatively low percentage error of 3.37%, compared with 14.57% for the del Valle-Aguilera model. These findings demonstrate the reliability of Chrastil's model in predicting the solubility of Sabah green coffee bean oil in SC-CO_2. Overall, the research highlights the potential of SC-CO_2 extraction as a sustainable, solvent-free approach for obtaining high-quality coffee oil extracts, with promising applications in the food industry and possible extension to the recovery of other bioactive compounds in food processing.

Keywords: caffeine; chlorogenic acid; Sabah green robusta coffee bean; solubility; supercritical carbon dioxide extraction

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1. Introduction

Coffee ranks among the most favored beverages and is one of the most extensively traded commodities. Statista projects that the global coffee market will grow by 3.01% from 2024 to 2029. In Malaysia, the coffee market is anticipated to expand by 1.43% during the

same period. Coffee belongs to the *Rubiaceae* family and the genus Coffea, originating from the tropical regions of Africa, particularly Ethiopia. There exist 124 species of coffee, with only two extensively cultivated and commercialized: *Coffea arabica* (Arabica) and *Coffea canephora* (Robusta) [1]. Arabica thrives in cooler climates (15–22 °C) and higher elevations (1000–2000 m), making it unsuitable for Malaysia's lower highlands [2]. The predominant coffee cultivated in Malaysia is robusta coffee.

In the 1900s, the coffee crop market experienced a drop due to leaf rust disease (*Hemileia vastatrix*) and the infestation of the clear wing moth (*Cephanodes hylas* L.). As of now, recent advancements in research and technology have resolved existing issues, resulting in increased production, positioning Malaysia as the 44th largest coffee exporter globally in 2022. According to the Department of Agriculture, Sabah has the largest coffee cultivation area, with approximately 1434.20 hectares; nevertheless, its production ranks second to Johor, with roughly 935.10 metric tonnes in 2022. Coffee is a significant commodity with potential for development driven by the need for value-added products. Given this upward trend, there is significant potential for value-added coffee products beyond traditional beverages, particularly coffee bean oil, which is gaining interest for applications in the cosmetic, pharmaceutical, and food industries [3,4].

Coffee oil is primarily composed of triacylglycerols and fatty acids, resembling the lipid composition of other edible vegetable oils. Green coffee oil, typically extracted via cold pressing, has a greenish-yellow hue and a mild aroma. Owing to its antioxidant and moisturizing properties, it is increasingly used in skincare and cosmetic formulations [1]. Recent research has also explored its suitability for oral formulations, driven by its health-promoting properties. Coffee and its derivatives have been associated with thermogenic effects, reduced oxidative stress, improved immune response, and potential therapeutic benefits for metabolic and neurodegenerative diseases such as diabetes, cardiovascular disorders, and Alzheimer's disease [3,5]. These benefits are largely attributed to its bioactive constituents—including caffeine, trigonelline, lipids, fatty acids, proteins, vitamins, and chlorogenic acid [4,6].

Among these, caffeine and chlorogenic acid are the most studied bioactive compounds, contributing significantly to coffee's health effects. Caffeine, a methylxanthine alkaloid, is the world's most widely consumed psychoactive compound [7]. Beyond its stimulant effects, emerging studies indicate its role in modulating oxidative and inflammatory pathways and delaying physiological decline with age [8]. Chlorogenic acid (5-caffeoylquinic acid), a polyphenolic ester formed from caffeic and quinic acids, has demonstrated therapeutic potential for managing type 2 diabetes, cardiovascular disease, and inflammation-related conditions [9]. More recently, it has also been explored for its neuroprotective effects against diseases such as neuropathic pain and Alzheimer's [10]. The combined effects of caffeine and chlorogenic acid position coffee as a promising raw material for functional food and nutraceutical applications.

Supercritical carbon dioxide (SC-CO_2) extraction is a novel clean technology utilized in the processing of food, cosmetic, and pharmaceutical products. SC-CO_2 extraction offers some recognized advantages compared to traditional methods [11]. Conventional extraction often relies on organic solvents that pose toxicity risks and may degrade thermolabile compounds at high temperatures. Carbon dioxide (CO_2), a non-flammable and non-toxic solvent, facilitates extraction operations under mild conditions owing to its relatively low critical constants (critical temperature, Tc = 31.1 °C and critical pressure, Pc = 7.3 MPa) [12–15]. As a gas at ambient pressure, CO_2 leaves no residual solvent in the final product, making SC-CO_2 ideal for producing clean, high-purity extracts with minimal thermal degradation [16]. Although SC-CO_2 extraction of coffee oil has been reported, there is limited research on the solubility behavior of coffee oil specifically from Malaysian

robusta beans, particularly in relation to bioactive retention and model-based process optimization. Most previous studies have focused on either yield or compound quantification without addressing the solubility modeling aspect, which is crucial for understanding extraction kinetics and scaling up the process.

This study advances previous work by generating new solubility data for Sabah green robusta coffee bean oil in SC-CO_2 under various temperature and pressure conditions. Importantly, it compares the predictive capabilities of two semi-empirical models—Chrastil [17] and del Valle–Aguilera [18] which are frequently used for solubility modeling in SC-CO_2 systems. Beyond their historical application, these models were chosen due to their relevance to the physicochemical properties of coffee oil, which is rich in neutral lipids. The Chrastil model, based on association theory, effectively correlates solubility with temperature and density changes. Meanwhile, the del Valle–Aguilera model, which incorporates solvent density and molecular descriptors, offers additional flexibility for multicomponent systems. By applying and comparing both models, this study not only predicts solubility behavior with high accuracy but also provides insights into solvent–solute interactions relevant for robusta coffee oil extraction.

2. Materials and Methods

2.1. Robusta Coffee Beans Preparation

The coffee fruit was collected in October 2022 from a farm in Tenom, Sabah, Malaysia. The beans were extricated from the fruits and subsequently sun-dried for a whole day until the moisture content reached approximately ±10%. The desiccated coffee beans were ground and screened to achieve a particle size of 300 µm. Subsequently, the beans were stored in a hermetically sealed bag and placed in a freezer kept at −20 °C to retain their freshness.

2.2. Supercritical Carbon Dioxide (SC-CO_2) Extraction

The extraction took place in a custom-built SC-CO_2 unit developed by Ruas Tech Sdn. Bhd., Malaysia. The SC-CO_2 unit was composed of a 200 mL extraction vessel designed to withstand a maximum pressure of approximately 40 MPa, a CO_2 plunger metering pump (SIKOPUMP, Shanghai, China), a heater controller (Nantong Wisdom SCFE, Jiangsu, China), a cooling water circulation system (BIOBASE, Shandong, China), various valves, and a pressure relief valve. The extraction process utilized 99.99% industrial grade carbon dioxide, CO_2, supplied by Syarikat Jaya Usaha in Kota Kinabalu, Sabah, Malaysia. Subsequently, approximately 20 g of ground coffee beans were accurately measured and placed into the extraction vessel. The CO_2 was first cooled to 6 °C and subsequently maintained at a steady flow rate of 1 L/hr. The dynamic SC-CO_2 extraction process was conducted at temperatures ranging from 40 to 80 °C and pressures between 10 and 30 MPa, over a duration of 3 h, as conducted by Putra et al. [19]. The coffee bean oil was gathered and documented at 15 min intervals, with solubility determined by the slope of the extraction curve and expressed in mg oil/g CO_2 utilized. After each extraction run, the system was flushed using ethanol to ensure thorough cleaning of the extraction vessel and associated lines.

2.3. Quantification of Caffeine and Chlorogenic Acid

High-performance liquid chromatography (HPLC) was used to identify and quantify caffeine and chlorogenic acid in the Sabah green robusta coffee bean extract using Fajara and Susanti [20] with slight modification. The HPLC system employed (Agilent Technologies, California, USA) was equipped with a model 1200 pump and a diode array detector (DAD) set at 274 nm. Separation was performed on a Shim-pack C18 column (15 cm × 4.6 mm, 5 µm particle size) coupled with an autosampler. An isocratic mobile phase consisting of

HPLC-grade methanol and water (80:20, *v*/*v*) was used at a flow rate of 1.0 mL/min. A 20 µL sample was injected into the column, and the column temperature was maintained at 40 °C throughout the analysis. The eluted compounds were monitored using the DAD at 274 nm, and the caffeine content in the samples was quantified based on the detector response. A standard was prepared with concentrations 20, 40, 60, 80 and 100 ppm. The calibration curve obtained was $Y = 43.025X + 400.67$ and a R^2 value of 0.9971 using caffeine as the standard. Another calibration curve was also obtained using chlorogenic acid as standard, $Y = 16.733X - 327.14$ and a R^2 value of 0.939. The amount will be quantified by comparing retention time of peaks in the sample in contrast to caffeine and chlorogenic acid standard peaks.

2.4. Solubility Determination and Correlation Model

Sabah green coffee bean oil was extracted using a dynamic extraction method. The experimental solubility of the solute was determined by calculating the constant extraction rate (CER) phase, represented by the initial slope of the extraction curve on a plot of solute concentration versus solvent consumption. Table 1 shows the variation in SC-CO_2 density with changes in temperature and pressure, ranging from 221 to 910 g/L. The corresponding density values of SC-CO_2 were obtained from The Engineering Toolbox database.

Table 1. The solubility data of Sabah green coffee bean oil.

Temperature (°C)	Pressure (MPa)	Solvent Density (g/L)	Yield (mg/g Sample)	Experimental Solubility (mg Extract/g Solvent)	Calculated Solubility-Chrastil (mg Extract/g Solvent)	Calculated Solubility-dVa (mg Extract/g Solvent)
80	10	221.6	18.20	0.542	0.543	0.542
60	10	290.0	26.07	0.559	0.573	0.512
40	10	628.7	44.60	0.948	0.948	0.661
80	20	594.1	46.57	0.440	0.439	0.665
60	20	723.8	44.43	0.444	0.536	0.661
40	20	839.9	49.13	0.656	0.656	0.656
80	30	746.0	86.13	1.727	1.727	1.926
60	30	830.0	96.93	2.167	2.131	2.167
40	30	910.0	101.20	2.681	2.682	2.488

To predict the solubility behavior of Sabah coffee bean oil in SC-CO_2, the experimental solubility data were correlated using two semi-empirical models. One of the earliest models, proposed by Chrastil [17], is based on the concept that, under supercritical conditions, solute and solvent molecules associate to form solvato-complexes at equilibrium. This concept gave rise to a model that relates solute solubility to the density of the pure solvent, as expressed in the following equation:

$$Y = \rho^k \exp\left(a + \frac{b}{T}\right) \quad (1)$$

where Y represents the solubility of the solute ($kg \cdot m^{-3}$), while ρ denotes the density of the supercritical fluid ($kg \cdot m^{-3}$). The parameter k is the association number, and a is a function of both the association number and the molecular weights of the solute and the supercritical fluid. The parameter b is related to the enthalpy of solvation and vaporization, whereas T denotes the temperature. The association constant (k) describes the dependence of solubility on fluid density, while the temperature effect on solubility is expressed through the parameter b.

Del Valle and Aguilera [18] proposed a modification to Chrastil's equation to incorporate the effect of temperature-dependent variations in the enthalpy of vaporization:

$$Y = \rho^k \exp\left(\frac{a}{T} + \frac{b}{T^2} + c\right) \quad (2)$$

where constants a and b reflect the influence of temperature on the solubilization process, whereas the constant c corresponds to the molecular weights of both the solute and the solvent.

2.5. Data Validation

Nonlinear regression data fitting was performed using the Solver tool in Microsoft Excel 2019, and the best-fitting models were evaluated based on the average absolute relative deviation ($AARD\%$):

$$AARD\% = \frac{1}{n}\sum_{i=1}^{n}\left|\frac{N_{exp} - N_{calc}}{N_{exp}}\right| \times 100\% \quad (3)$$

where n denotes the number of data points, N_{exp} represents the experimental values, and N_{calc} refers to the values calculated from the models.

3. Results and Discussion

3.1. Extraction of Sabah Green Coffee Bean Oil

Figure 1 illustrates the effect of SC-CO_2 extraction pressures (10, 20, 30 MPa) and temperatures (40, 60, 80 °C) on the yield of Sabah green coffee bean oil, which expressed as mg/g sample. The increasing trend of the oil yield with an increase in pressure at extraction pressures 10 to 30 MPa at constant temperature was observed. For example, the coffee bean oil yield increased from 44.60 to 101.20 mg/g sample at constant temperature of 40 °C, indicating that higher the pressures enhance the extraction efficiency. This increasing trend can be explained by the fact that elevated pressure increases CO_2 density, which enhances its solvating power. In the supercritical state, CO_2 behaves like a dense fluid, and greater density translates to better ability to dissolve and carry non-polar compounds like lipids and oils [21]. This behavior is consistent across all three temperature levels tested, confirming that pressure is a dominant factor in enhancing extraction yield under SC-CO_2 conditions.

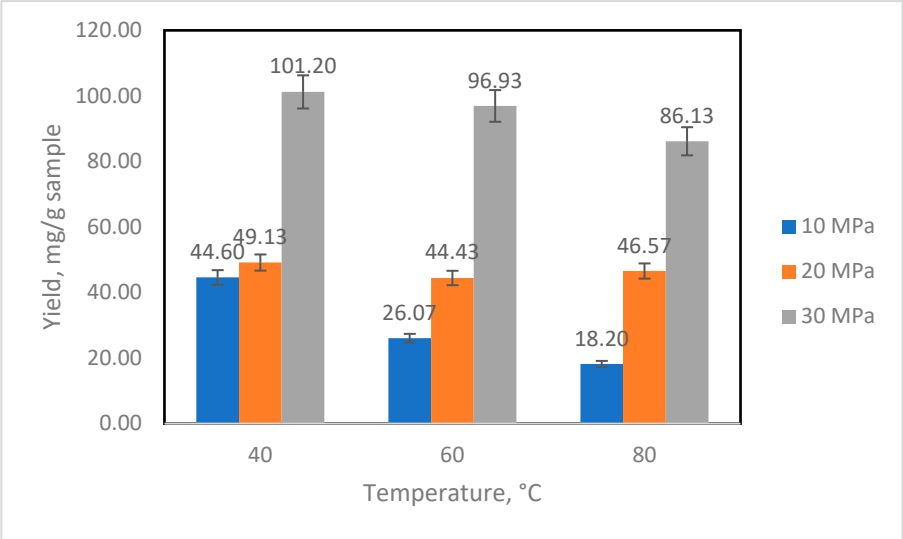

Figure 1. Effect of SC-CO_2 extraction conditions on the Sabah green coffee beans oil.

In contrast the effect of temperature shows an opposite trend: as temperature increased from 40 to 80 °C at constant pressure, oil yield generally decreased. For instance, at 10 MPa, the oil yield declined from 44.60 mg/g sample at 40 °C to 18.20 mg/g sample at 80 °C. This reduction may be attributed to the reduction in CO_2 density at elevated temperatures, which weakens its solvating power, even though higher temperatures may increase solute vapor pressure and improve mass transfer [21]. Hence, the negative impact of reduced solvent density outweighs the benefits of improved diffusion.

The highest oil yield of 101.20 mg/g sample was obtained at the lowest temperature of 40 °C and highest pressure of 30 MPa, which represents the optimal condition for oil extraction under the parameters tested. Conversely, the lowest yield of 18.20 mg/g sample was observed at 10 MPa and 80 °C, highlighting the compounded negative effect of low pressure and high temperature.

Caffeine and chlorogenic acid are two major compounds found in coffee beans that influence not only flavor and aroma but also offer notable health benefits. In this study, Sabah green coffee beans were extracted and analyzed to assess the content of caffeine and chlorogenic acid using HPLC. The experimental results for the caffeine and chlorogenic acid analysis in Sabah green coffee bean samples are presented in Figures 2 and 3, respectively. Figure 2 shows that caffeine content varied significantly across different conditions. The maximum caffeine concentration of 22.713 mg/g was obtained at 80 °C and 10 MPa, suggesting that high temperatures facilitate the diffusion of caffeine molecules due to increased vapor pressure. At this temperature, the kinetic energy of molecules increases, enhancing mass transfer and release from the solid matrix [22]. However, as pressure increased to 30 MPa, caffeine content decreased to 11.441 mg/g, indicating that high CO_2 density may hinder caffeine solubility due to reduced diffusivity in the solvent phase [23].

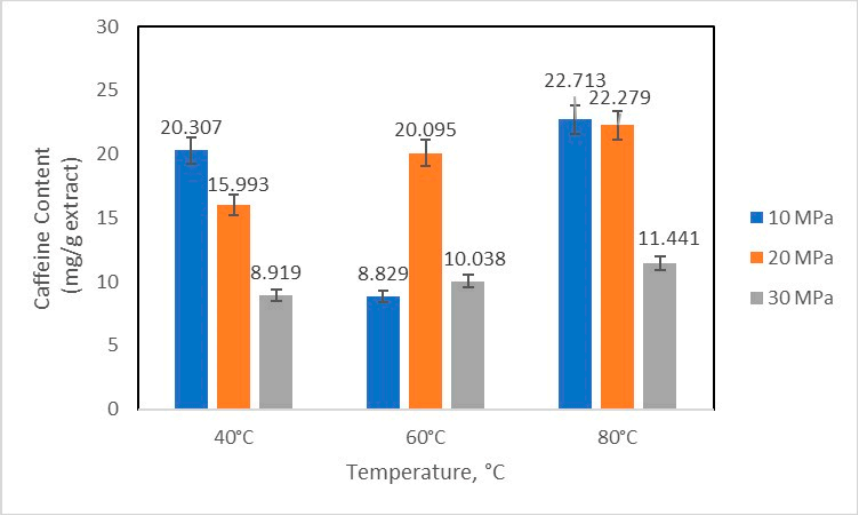

Figure 2. Effect of SC-CO_2 extraction conditions on the caffeine content extracted from Sabah green coffee beans oil.

Figure 3 highlights the extraction behavior of chlorogenic acid, a polyphenolic compound that is more thermolabile and polar compared to caffeine. The highest chlorogenic acid content of 0.984 mg/g extract was recorded at 80 °C and 10 MPa, indicating that similar to caffeine, higher temperatures promote release, possibly by breaking cell wall matrices. However, chlorogenic acid is more susceptible to degradation at high temperatures [24]. Its solubility decreased with increasing pressure and temperature, likely due to both thermal degradation and lower affinity for CO_2 [21]. As pressure increased, the chlorogenic acid content declined sharply. At 80 °C and 30 MPa, its concentration dropped to 0.673 mg/g extract, likely due to both thermal degradation and reduced compatibility with denser CO_2.

At 60 °C and 30 MPa, it was only 0.261 mg/g, reinforcing that higher pressures are not favorable for extracting this compound.

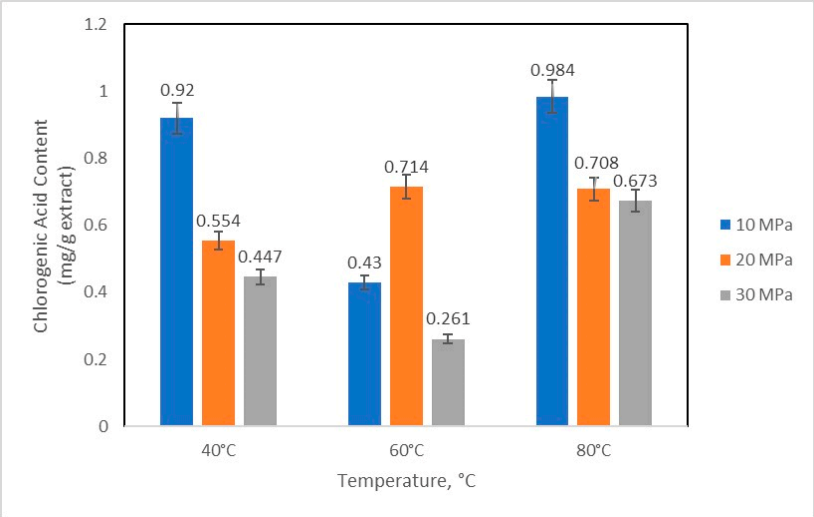

Figure 3. Effect of SC-CO_2 extraction conditions on the chlorogenic acid content extracted from Sabah green coffee beans oil.

Overall, caffeine content ranged from 8.829 to 22.713 mg/g while chlorogenic acid concentrations ranged from 0.261 to 0.984 mg/g extract. Notably, while both caffeine and chlorogenic acid showed maximum recovery at 80 °C and 10 MPa, the rapid decline in yield for chlorogenic acid at higher pressures and temperatures points to a narrower optimal window for its stable extraction. These results underline the need for carefully controlled extraction conditions when targeting sensitive bioactive compounds.

In summary, the behaviors shown in Figures 1–3 underscore the complex interaction between temperature and pressure in SC-CO_2 extraction. While higher pressures improve extraction of oils by increasing CO_2 density, they may negatively affect the extraction of polar or thermolabile compounds like caffeine and chlorogenic acid. Likewise, elevated temperatures may enhance mass transfer but reduce CO_2 solvent power or induce compound degradation. Therefore, the extraction conditions must be tailored according to the physicochemical nature of target compounds to optimize yield and selectivity [21,25].

3.2. Solubility of Sabah Green Coffee Bean Oil

Solubility data are a critical parameter in SC-CO_2 extraction, guiding the selection of optimal conditions for efficient recovery of targeted compounds. Table 1 and Figure 4 summarize the solubility of Sabah green coffee bean oil under various temperature and pressure conditions, with values ranging from 0.440 to 2.681 mg/g CO_2. The solubility was evaluated at pressures of 10, 20, and 30 MPa and temperatures of 40, 60, and 80 °C.

Figure 4 shows that at constant pressure, the solubility of Sabah green coffee bean oil decreases as temperature increases from 40 to 80 °C. For instance, at 10 MPa, solubility declined from 0.948 mg/g at 40 °C to 0.542 mg/g at 80 °C, while at 30 MPa, it decreased from 2.681 mg/g at 40 °C to 1.727 mg/g at 80 °C. This trend is primarily attributed to the reduction in SC-CO_2 density at elevated temperatures, which lowers its solvating power. Although higher temperatures enhance the vapor pressure of the solute and could improve mass transfer, the effect is often outweighed by the decrease in solvent density, leading to reduced solubility. For example, Brunner [26] documented that solubility tends to decrease with rising temperature at pressures below the so-called crossover point, due to reduced solvent density overpowering the vapor pressure effect. Similar observations were reported by Özkal et al. [27] in their work on apricot kernel oil, and Maheshwari et al. [28]

in studies on fatty acids, reported that at pressures below the crossover threshold around 20–30 MPa, solubility typically declines with temperature due to the dominant effect of declining CO_2 density.

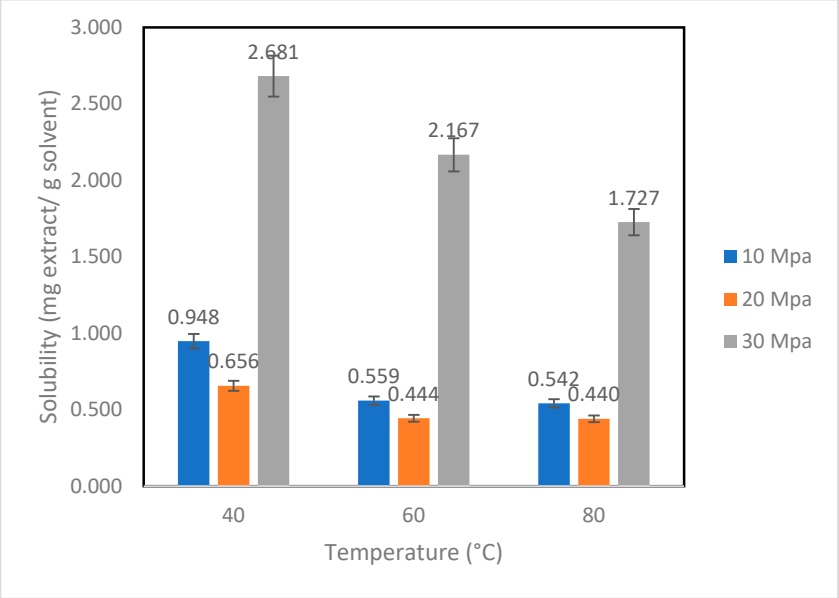

Figure 4. Effect of the SC-CO_2 extraction conditions on the solubility of Sabah green coffee bean oil.

Conversely, at constant temperature, solubility exhibits a nonlinear relationship with pressure. At 40 °C, solubility decreased from 0.948 mg/g at 10 MPa to 0.656 mg/g at 20 MPa but then increased substantially to 2.681 mg/g at 30 MPa. A similar pattern was observed at 60 °C and 80 °C, where solubility declined slightly at 10 MPa to 20 MPa, before rising again at 30 MPa. This non-monotonic trend suggests that the increase in pressure from 10 to 20 MPa was insufficient to significantly raise CO_2 density and improve solubility, possibly due to mass transfer limitations or weaker solvent–solute interactions in that pressure range [26,29]. However, the further increase to 30 MPa results in a notable rise in solvent density, which enhances solute–solvent affinity and extraction efficiency [30].

Furthermore, while increasing temperature tends to raise the vapor pressure of solutes where favoring solubility and it also decreases the density of SC-CO_2, which reduces its solvating power. At low to moderate pressures, the reduction in solvent density outweighs the vapor pressure effect, resulting in decreased solubility [27,28]. This interplay between pressure, temperature, and solubility reflects the typical "crossover" behavior where at lower pressures, the decrease in solvent density due to increasing temperature outweighs the rise in solute vapor pressure, reducing solubility. However, at pressures above the crossover point (~25–30 MPa), the density remains high enough that solubility may plateau or even increase with temperature. This behavior is typical in SC-CO_2 systems and underscores the importance of selecting appropriate pressure-temperature combinations.

The solubility behavior is strongly tied to the chemical nature of the extracted compounds. CO_2 is a non-polar solvent, making it effective for dissolving non-polar or slightly polar compounds such as triglycerides and fatty acids, which constitute the major components of green coffee bean oil [26,27]. At lower temperatures, CO_2 exhibits higher density, allowing for more effective van der Waals interactions with non-polar solutes. As temperature increases, the weakening of these interactions contributes to the observed decrease in solubility, especially at lower pressures [28,31]. However, at sufficiently high pressures, the density of CO_2 remains adequate even at elevated temperatures, maintaining or improving solubility—consistent with crossover pressure behavior [26].

Additionally, the presence of minor polar compounds such as chlorogenic acid can further influence solubility through dipole interactions and hydrogen bonding. Although SC-CO_2 is generally non-polar, its extraction capability for polar compounds can be enhanced through the addition of co-solvents like ethanol. Research has shown that co-solvent-assisted SC-CO_2 extraction can improve the recovery of polar bioactives, a strategy worth investigating for improving the yield of functional components from green coffee beans [31,32].

3.3. Correlation Data of Sabah Green Coffee Bean Oil

The solubility data of Sabah green coffee bean oil in SC-CO_2 were correlated using two established semi-empirical models: the Chrastil model and the del Valle and Aguilera model. Table 2 presents the results of these correlations. Both models were applied to the experimental solubility data using Microsoft Excel 2007 Solver by minimizing the *AARD*% to determine the fitting parameters.

Table 2. Coefficient parameter and *AARD*% for Chrastil and del-Valle Aguilera model on the solubility of Sabah green coffee bean oil.

Models	Model Constants	Model Coefficient
Chrastil	k	0.510
	a	228.977
	b	−3.912
	AARD%	3.37
Del Valle-Aguilera	k	0.169
	a	−214.975
	b	−3.912
	c	−0.357
	AARD%	14.57

In the Chrastil model, parameters a, b, and k hold physical significance: a corresponds to the combined heat of solvation and vaporization of the solute, b represents the molecular characteristics such as molecular weight and melting point, and k denotes the number of CO_2 molecules associated with each solute molecule in the solvate complex [17]. The *AARD*% obtained from this model was 3.37%, indicating a strong correlation with the experimental data. The del Valle and Aguilera model, which includes an additional parameter c to account for temperature-dependent changes in solute vaporization enthalpy [18], resulted in a higher *AARD*% of 14.57%, reflecting a less accurate fit. While the model is more adaptable for systems with strong temperature dependence, its performance was inferior for Sabah green coffee bean oil, likely due to the lipid-rich, non-polar nature of the solute.

These findings are consistent with prior studies. For instance, Zuknik et al. [33] compared the two models in modeling the solubility of virgin coconut oil in SC-CO_2 between 40 and 80 °C and 20.7 and 34.5 MPa. The del Valle and Aguilera model slightly outperformed the Chrastil model, with an *AARD*% of 0.39% versus 0.93%, respectively. Nevertheless, both models were deemed effective in representing the experimental data. Similarly, Duba and Fiori [34] evaluated the solubility of grape seed oil in SC-CO_2 using both models under pressures ranging from 15 to 35 MPa and temperatures between 40 and 70 °C. They reported that the Chrastil model better represented the experimental data, especially at higher pressures, with *AARD*% values around 2.8%, compared to 5.4% for the del Valle and Aguilera model. The study concluded that Chrastil's model was more robust in systems dominated by van der Waals interactions, such as lipid-rich matrices.

Thus, the results of this study reaffirm that the Chrastil model provides a more reliable and accurate representation of the solubility behavior of Sabah green coffee bean oil in SC-CO_2 under the tested conditions, particularly due to its compatibility with the solute's non-polar character and the extraction mechanism driven by solvation complex formation.

4. Conclusions

Sabah green coffee bean oil was successfully extracted using supercritical carbon dioxide (SC-CO_2) across a range of temperatures (40–80 °C) and pressures (10–30 MPa). The extraction process yielded a higher concentration of caffeine (22.713 mg/g extract) compared to chlorogenic acid (0.984 mg/g extract), with the highest overall oil yield obtained at 10 MPa and 80 °C. Solubility of the oil in SC-CO_2 varied from 0.440 to 2.681 mg/g solvent, reaching a maximum at 30 MPa and 40 °C. Among the solubility models tested, the Chrastil model provided the best correlation with experimental data, achieving a low average absolute relative deviation (*AARD*%) of 3.37%, indicating strong predictive reliability. These results demonstrate the potential of SC-CO_2 as an environmentally friendly and selective method for extracting bioactive-rich oil from Sabah green coffee beans. The high solubility values and effective recovery of chlorogenic acid suggest that this technique is suitable for producing functional ingredients. However, this study was limited to the analysis of caffeine and chlorogenic acid, excluding other potentially valuable bioactive compounds. Moreover, the extraction was carried out at laboratory scale, and its feasibility for industrial-scale application remains unexamined. The stability of the extracted oil was also not assessed, although it is a critical factor for its incorporation into functional formulations. While the Chrastil model exhibited strong predictive performance, the findings presented here are specific to Sabah green coffee beans and may not directly apply to other coffee varieties.

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Conflicts of Interest: The authors declare no conflicts of interest.

Abbreviations

The following abbreviations are used in this manuscript:

SC-CO_2	Supercritical Carbon Dioxide Extraction
CO_2	Carbon Dioxide
HPLC	High-Performance Liquid Chromatography
CER	Constant Extraction Rate
AARD%	Average Absolute Relative Deviation

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