

Empirical modelling, simulation and control of coffee brewing

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Abstract

Coffee brewing is a complex process governed by various parameters, such as water temperature, extraction time, and particle size of ground coffee. These parameters affect the quality of brewed coffee in terms of flavour and intensity of aromatic compounds. This research focused on studying the effect of water temperature on caffeine concentration in brewed coffee. This was done by varying the water temperature (80°C, 85°C and 90°C) in infusion coffee brewing while keeping other parameters such as coffee type (Arabica), coffee particle size (500 µm), and coffee-to-water ratio constant. The results showed that the concentration of caffeine in the brewed coffee increased as the water temperature increased, with the highest concentration observed at 90°C with 210.58 g/L. An empirical model, represented as a first-order model with time delay (FOPTD), was developed to study the effect of temperature in the brewing process. The model was then simulated and controlled using a Proportional Integral (PI) controller tuned using different methods. Performance and robustness analysis were conducted, and the best results were obtained using the fractional-order controller with an Integral of Absolute Error (IAE) of 64.67. In conclusion, the effect of water temperature on caffeine concentration during coffee brewing was determined, and a brewing model at different water temperatures was developed and simulated with different tuning rules for the PI controller.

1. Introduction

World coffee consumption increased by 1% (165.4 million bags) in the year 2020/2021 as the global economy recovered from the pandemic in the year 2019. Asia and Oceania showed the fastest growth rate, with a 9.1% increase in coffee consumption compared to other regions worldwide (International Coffee Organization [ICO], 2021). This trend indicates enormous potential for the coffee industry in the future. In Malaysia, coffee enthusiasts are transforming their passion into a feasible business (Azavedo and Gogatz, 2021), promoting the coffee-drinking culture in the community.

There are more than 66 species of coffee, but two of the most commonly cultivated species worldwide are Arabica and Robusta coffee. However, in Malaysia, Robusta, and Liberica coffee are commonly grown by coffee planters (Khazanah Research Institute, 2019). The challenge is that Liberica coffee is more accepted locally compared to worldwide, which has caused the price of Liberica coffee to be lower in the world market. However, these green coffee beans (Robusta and

Liberica coffee) are further processed into higher value-added coffee products through Malaysia's growing food and beverage manufacturing industry. On the other hand, Arabica coffee is referred to as high grade, with complexity in flavours and aromas, making it in high demand worldwide.

Generally, coffee extraction starts with water absorbing into the ground coffee, followed by the mass transfer of soluble compounds from the ground coffee into hot water, and then separating the extracting coffee solids (Petracco, 2008; Wang *et al.*, 2016). The extraction process involves different parameters depending on the brewing methods. The three main categories of coffee extraction are the decoction method (boiled coffee, Turkish coffee, percolator coffee, and vacuum coffee), the infusion method (filter coffee and *Napoletana*) and the pressure method (Plunger, Moka, and espresso). Brewing methods are very important in determining the quality of coffee, especially among coffee lovers.

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Infusion is the most common brewing method, as it is an easy and economical process. The force from hot water that leaches to ground coffee is extracting a gentle taste and appropriate coffee oils and caffeine. However, due to shorter contact times, beverages are sensorily assessed as milder, often enhancing coffee's acidity and flavour (Petracco, 2008). Coffee extraction parameters such as extraction time, water temperature, pressure, particle size, coffee-to-water ratio, and water quality have a significant impact on the coffee flavour (Cordoba *et al.*, 2020).

The water temperature is the driving force that extracts chemical compounds from coffee grounds. At higher temperatures, the kinetic energy of water molecules is higher, and they move faster at every position compared to lower temperatures (Mestdagh *et al.*, 2017). The temperature will also affect the solubility. For instance, a higher temperature can increase the solubility of many compounds, resulting in higher volatility of chemical release (Angeloni *et al.*, 2019). The total solids and caffeine content are higher when using a brewing water temperature of 110°C (Albanese *et al.*, 2009). Low temperatures can only produce low concentration, extraction percentage, and total solids (Angeloni *et al.*, 2019).

Previous studies showed that using gradient temperature profiles such as from 88°C to 93°C had resulted in an increase of caffeine, less acidic compounds, and chlorogenic acid extraction (Salamanca *et al.*, 2017). Hot coffee brews contain higher concentrations of total acids that can be titrated and higher antioxidant activity than cold brew coffees (5°C to 30°C). Hot brewing methods extract more non-deprotonated acids than cold brew methods (Rao and Fuller, 2018). Studies also stated the difference between cold brewed coffee when prepared at 25°C and 4°C. A higher concentration of total solids, caffeine, total caffeoylquinic acids (CQAs), and 5-CQA concentrations is present in cold brews at 25°C than those brewed at 4°C (Angeloni *et al.*, 2019). Cold brew coffee has intense sweetness, fruity and floral flavours, medium bitterness and acidity, and a creamy body (Cordoba *et al.*, 2021). Odor-active compounds such as furans, pyrazines, ketones, aldehydes, pyrroles, esters, lactones, furanone, and phenols have also been identified in these coffee brews (Cordoba *et al.*, 2019).

In addition, the brewed water temperature will affect the saturated vapour pressure of aromatic compounds. High water temperature leads to the evaporation of volatile organic compounds (López *et al.*, 2016). For instance, volatile compounds such as guaiacol and pyrazines are present in coffee beverages made using high-temperature water of more than 96°C. These

compounds can release smoky, nutty, hazelnut-like, and roasty sensory notes (Caporaso *et al.*, 2014). In contrast, a significant reduction in furan compounds is observed when high water temperatures (near 100°C) are used (la Pera *et al.*, 2009).

The complexity of coffee brewing has triggered the development of various dynamic mathematical models to replicate the process. A multiscale model was proposed by Moroney, *et al.* (2015) that describes the coffee extraction by hot water from a bed of coffee grains that consist of different types of porosity. The study has initiated more models being developed which demonstrate the hydrodynamic and molecular dynamic (Ellero and Navarini, 2019) and the transport of dissolved substances such as caffeine and chlorogenic acids (Giacomini *et al.*, 2020) during the coffee extraction process. On the other hand, Cameron *et al.* (2020) proposed a combination of the dynamic model with the reaction kinetic (experimental) model and improvements were made using sensory study. Though these reported models were able to describe the behaviour of coffee brewing effectively, it is time-consuming due to the numerous parameters involved and the convoluted relationship.

Therefore, the purpose of the present study was to develop an empirical model for simulation and control of coffee brewing. An infusion brewing method was selected as it allows full extraction of flavours, and consistent results, and being preferred by many coffee lovers.

2. Materials and methods

2.1 Experimental analysis

Roasted Arabica (Brazil) coffee beans were purchased from Mister Coffee Sdn. Bhd., a local coffee roastery in Malaysia. The coffee beans were grounded (particle size of 500 µm) for an infusion method of coffee brewing. The water temperature used for brewing was varied at 80°C, 85°C and 90°C. The extracted coffee was taken for caffeine concentration analysis. Caffeine analysis was done according to the specification of Malaysian Standard (MS) 1235:1991 using High-Performance Liquid Chromatography (HPLC).

2.2 Model identification

An approximation of the parameter transfer function from the experimental response can be obtained by fitting the experimental response with the general first-order with time delay (FOPTD) model. The experimental data were analysed in the graphical form in Microsoft Excel. A first-order system can approximate the parameter with transport lag. The parameter values of

process gain (K), time constant (τ), and time delay (θ) are identified for the process.

The transfer function for FOPTD is shown in Equation 1.

$$G(s) = \frac{K e^{-\theta s}}{\tau s + 1} \quad (1)$$

The process gain can be obtained by simply calculating the ratio of the steady-state change to the input change. The value of process gain (K) is shown in below Equation 2 (Seborg *et al.*, 2016).

$$K = \frac{\Delta \text{Output}}{\Delta \text{Input}} = \frac{\Delta \text{Concentration}}{\Delta \text{Temperature}} \quad (2)$$

2.3 Time constant and time delay

The time constant is obtained by determining the corresponding time at 63.2% from the steady-state concentration and minus the dead time. The value of the time constant indicates the rate of response (Method 1) as shown in Equation 3.

$$\tau = \tau_{63.2\%} - \theta \quad (3)$$

Where θ is time delay.

Another method to calculate the time constant and time delay was proposed by Sundaresan and Krishnaswamy (1978) which avoids using inflexion point construction. The time delay and time constant will be obtained by corresponding the response time of t_1 and t_2 at 35.3% and 85.3%, respectively. The following Equation 4 and Equation 5 are used to determine the time delay (θ) and time constant (τ), respectively (Method 2).

$$\theta = 1.3t_1 - 0.29t_2 \quad (4)$$

$$\tau = 0.67(t_2 - t_1) \quad (5)$$

The root means square error (RMSE) is used to find out the best-fitting model from the experimental data, at both Method 1 and Method 2. The RMSE is given by below Equation 6.

$$\text{RMSE} = \sqrt{\frac{1}{N} \sum (x_{\text{actual}} - x_{\text{model}})^2} \quad (6)$$

2.4 Simulation and control

The control setting was introduced into a closed-loop system to ensure desired dynamic and steady-state response characteristics. Proportional integral derivative (PID) controller modes were used in this study. Three different tuning methods were used; the classical Ziegler-Nichols method, Chen *et al.* (2008) method, the Internal Model Control (IMC) method and fractional-order method and the optimum tuning method (Seborg *et al.*, 2016) (Gude and Kahoraho, 2009).

2.4.1 Ziegler-Nichols method

Ziegler and Nichols proposed the classical tuning method PID controller in the early 1940s. There were two types of methods that Ziegler-Nichols proposed. The first method is known as the continuous cycling method. This response is typically used for first-order systems with transportation delays. The PI controller parameters: proportional gain (K_p), and integral time (τ_i) can be calculated using Equation 7 and Equation 8 (Kushwah and Patra, 2014).

$$K_p = \frac{0.9\tau}{\theta} \quad (7)$$

$$\tau_i = \frac{\theta}{0.3} \quad (8)$$

This tuning method was also implemented in the hot-water dispenser system to maintain the water temperature (Aisuwarya and Hidayati, 2019).

2.4.2 Internal model control method

Garcia and Morari first introduced internal model control (IMC). The process model contains the internal part of the controller. The benefit of the IMC design method is that the controller parameters can be expressed directly into system parameters and the desired closed loop. Hence, the design procedure is simple. However, this may have lower parameter sensitivity risking oscillatory behaviour. For PI controller, the parameters were calculated using Equation 9 and Equation 10 (Bequette, 1999).

$$K_c = \frac{\tau_p}{K_p(\tau_c + \theta)} \quad (9)$$

$$\tau_I = \tau_p \quad (10)$$

2.4.3 Fractional-order method

The process parameter for PID controller is constantly updated in the process industry, which has posed challenges for control engineers. Ensuring the proper performance of the process requires careful selection of PID parameter tuning methods, as conventional PID tuning methods may not be sufficient to handle the complexities of modern industry processes. To achieve better control, studies on fractional-order with an additional degree of freedom tuning rules for stable FOPTD were compared (Ranganayakulu *et al.*, 2016). The controller transfer function is given by Equation 11.

$$G_c(s) = K_c \left(1 + \frac{1}{\tau_I s^\lambda} \right) = K_p + \frac{K_I}{s^\lambda} \quad (11)$$

2.4.3.1 Chen *et al.* (2008) method

In Chen *et al.* (2008), the tuning was considered

optimum when it could achieve set points quickly, and the load disturbance rejection was optimized. The fractional-order of the integral part (λ) depends on the value of the controller time constant. The value for controller gain (K_c) and integral time (τ_i) are shown in below Equation 12 and Equation 13 (Chen *et al.*, 2008).

$$K_c = \frac{1}{K} \frac{0.2978}{\tau_c + 0.000307} \quad (12)$$

$$\tau_i = \tau_c \left(\frac{0.8578}{\tau_c^2 - 3.402\tau_c + 2.405} \right) \quad (13)$$

2.4.3.2 Gude and Kahoraho method

In the Gude and Kahoraho method (2009), the tuning was considered optimum as it avoids overshoot, and the load disturbance rejection was optimized. The fractional-order of the integral part (λ) value is chosen to be 1.12 because the following order will give the FOPTD model. The value for controller gain (K_c) and integral time (τ_i) were calculated based on below Equation 14 and Equation 15.

$$K_c = \frac{1}{K} (a\tau^b + c) \quad (14)$$

$$\tau_i = \tau_p (a\tau^b + c) \quad (15)$$

2.5 Performance and robustness analysis

The performance was quantified using Integral Absolute Error (IAE). In the current study, the IAE criterion was chosen as a performance metric for the controller because the minimization of IAE results in slight overshoot and low settling time in the system's closed-loop response when there is a step-change in setpoint or load disturbance (Ranganayakulu *et al.*, 2016).

Meanwhile, the robustness was measured using phase and gain margin by plotting the bode plot in MATLAB.

3. Results and discussion

3.1 Effect of brewing temperature on the coffee concentration

3.1.1 Caffeine concentration

The trendline of caffeine concentration in the coffee brew at various temperatures is shown in Figure 1. The concentration of caffeine in coffee brews increases as the temperature increases. The result was supported by Olechno *et al.* (2021) who reported that temperature and pressure affect the caffeine concentration. On the other hand, Ellero and Navarini (2019) reported that the caffeine concentration had increased with the increase in the coffee extraction ratio (%). This also relates to the current result as the extraction ratio was largely affected by the water temperature during brewing. The

concentration trendline of coffee brew at various temperatures has a higher value of R^2 , which is 0.9371 with an exponential line. Equation 16 correlates caffeine concentration (y) for various water temperatures (x).

$$y = 33.981e^{0.0201x} \quad (16)$$

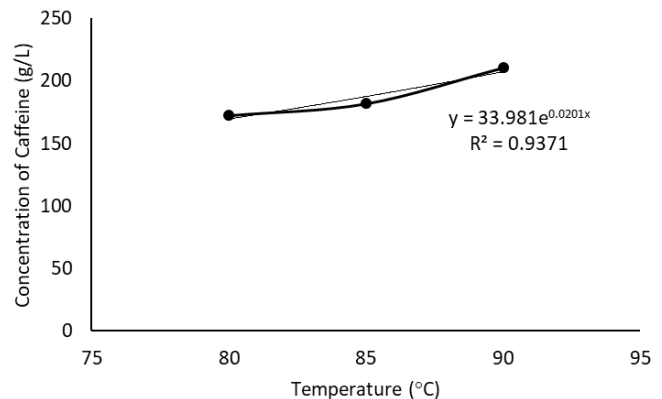


Figure 1. Trendline for caffeine concentration at various temperatures.

3.1.2 Coffee concentration profile

The term 'coffee concentration' refers to the amount of coffee solids extracted in a given amount of liquid (brewed coffee). 'Coffee concentration' is more general as compared to caffeine concentration (in 3.1.1) which is specific to the caffeine compound in coffee. Coffee concentration at the initial time is considered zero because no coffee is extracted into the solution and the water concentration is 0 g/L. In comparison, the coffee concentration at the final time of coffee brew at 80°C is 30.94 g/L, 85°C is 28.05 g/L, and at 90°C is 21.45 g/L. The concentration of coffee increases along with time (Figure 2), which corresponds to the finding that temperature affects the solubility of compounds. Higher temperature increases the solubility of compounds, resulting in higher release of chemicals (Angeloni *et al.*, 2019). At one point, the coffee concentration reaches a constant level from the 210s, indicating that the brewed coffee achieves an equilibrium condition or steady-state diffusion. Coffee soluble is diffused in and out at the

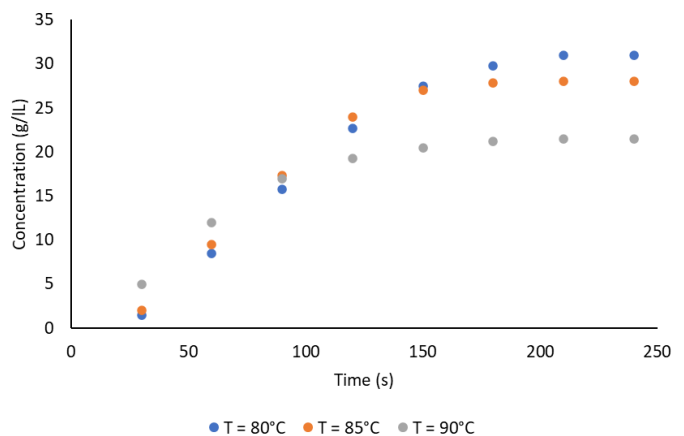


Figure 2. The concentration of brewed coffee at various temperatures during brewing.

same concentration (Moroney *et al.*, 2015).

3.2 Development of empirical models

Two methods were used to determine the first-order model with time delay (FOPTD): the estimation method and the equation method. The results are shown in Table 1. Based on these two methods, the process gain value is constant. The higher the concentration of coffee brew, the higher the value of process gain. In contrast, the higher the temperature value, the lower the value of process gain (Seborg *et al.*, 2016). Additionally, the value of the time delay will affect the value of the time constant. As the time delay increases, the time constant eventually decreases. The time delay is estimated to be lower in Method 1, while, the value is higher using Method 2. Table 1 also shows that the values of process gain decrease with increasing temperature from 80°C to 90°C. Similarly, other values also decrease with increasing water temperature for both methods.

Table 1. Transfer function of coffee brewing at three water temperatures; 80°C, 85°C, and 90°C.

		Method 1	Method 2
80°C	$K_p K_p$ (g/L °C)	0.39	0.39
	$\tau_p \tau_p$ (s)	70	47
	$\theta_p \theta_p$ (s)	25	50
85°C	$K_p K_p$ (g/L °C)	0.33	0.33
	$\tau_p \tau_p$ (s)	59	42
	$\theta_p \theta_p$ (s)	23	43
90°C	$K_p K_p$ (g/L °C)	0.25	0.25
	$\tau_p \tau_p$ (s)	50	40
	$\theta_p \theta_p$ (s)	10	23

The initial concentration at 90°C is higher than the other two temperatures and the first to achieve steady-state conditions. At the end of extraction, the concentration at 90°C was the lowest compared to 80°C and 85°C. This finding contrasted with the previous study as reported by Cai *et al.* (2022) that the concentration of coffee should be higher in higher temperatures as the kinetic energy is high. The high temperature increased mobility, and the possibility of leaching out compounds from the coffee bed due to higher physical forces (Mestdagh *et al.*, 2017). Nevertheless, it was found in this study that the optimum condition for infusion coffee brewing was at 80°C with

the highest soluble compound. This finding could be due to the higher water temperature of infusion coffee brewing at 90°C has caused the volatile compounds to be lost in the environment than at lower temperatures. The brewing equipment was exposed to other environmental factors which could not be controlled in the study.

Table 2 shows the values of RMSE for both methods (Method 1 and 2) to find the best-fitted first-order model plus time delay. RMSE was the most crucial criterion for model prediction, which was a good measure of how

Table 2. Root Mean Square Error (RMSE) for Method 1 and Method 2 at various water temperatures.

Temperature (°C)	Method 1	Method 2
80	21.416	21.418
85	20.602	20.603
90	20.654	20.646

accurately the model predicts the response. A lower value of RMSE indicates that the model has a better fit with experimental data. It was found that Method 1 has a lower RMSE value than Method 2 in temperatures 80 and 85°C, meanwhile, Method 1 has a higher RMSE value than Method 2 at 90°C. The most negligible value of RMSE is a model at 85°C for Method 1 with 20.602. This coffee brewing model can be used for the process control simulation.

3.3 Simulation and control of coffee brewing

The model used for simulation was the variable in Method 1 at 85°C coffee brew plant in a close-loop system with various tuning PI controller. Based on below Table 3, the value of K_c and τ_l was calculated and compared with different tuning rules. As the value used for PI controller in Matlab, the values of P and I were calculated based on the value of K_c and τ_l . The unit for K_c is a standard dimensionless (%/%).

3.3.1 Performance analysis

The fractional-order controller proposed by Chen *et al.* (2008), provides better performance with a lower value of IAE is 64.67. This indicates that the error calculated was minimal in this type of controller, resulting in faster settling time and rise time

Table 3. PI controller performance for various tuning rules from Simulink/Matlab.

Tuning Rule	Ziegler-Nichols	Internal Model Control (IMC)	Fractional-Order	
			Chen <i>et al.</i> (2008) method	Gude and Kahoraho method
IAE (cm ²)	80.94	92.48	64.67	105.3
Rise Time (s)	147	183	36.2	374
Settling time (s)	353	401	260	803
Overshoot (%)	0	0	25.7	0
Peak (no unit)	1	1	1.26	1

(Ranganayakulu *et al.*, 2016). The faster rise time and settling time mean quicker attainment of the setpoint compared to the other tuning rules. However, there was some overshoot with a value of 25.7%, whereas Ziegler-Nichols, IMC, and the fractional-order controller by Gude and Kahoraho (2009) have zero overshoot percentage. The peak value of overshoot was 1.26%.

On the other hand, the fractional-order controller by Gude and Kahoraho (2009) showed the lowest performance, with a higher value of IAE at 109.1. The rise time and settling time are slower in achieving the setpoint compared to the other tuning rules. However, there was no value of overshoot percentage, and the peak value is 1.

The second-best performing controller was the Ziegler-Nichols method, with a slightly higher value of IAE, rise time, and settling time compared to the fractional-order by Chen *et al.* (2008), followed by the IMC controller.

3.3.2 Robustness

The stability of tuning for the closed-loop system depends on the values of gain and phase margin. The parameter values shown in Table 4 demonstrate that positive gain margin and phase margin result in a stable closed-loop system. Previous studies have reported that the desired value of phase margin was between 30 to 60 degrees and the gain margin was between 2 to 10 dB (Kim, 2017). The best robust controller, according to Chen *et al.* (2008), was a fractional-order controller that falls within the desired value range, with a phase margin of 43.3 degrees and a gain margin of 9.2 dB. Other types of controllers were found to be outside the desired range for phase and gain margin.

A controller system must be stable in order to design an effective control system. An unstable response can result in input oscillations that do not diminish or become more significant. The stability of a system was measured based on the phase margin and gain margin obtained from the bode plot and frequency response. Phase and gain margins are values that indicate closed-loop stability. Generally, as the gain margin of a system increases, the system becomes less stable. The gain margin and the phase margin indicate how much the gain increases until the system becomes unstable.

The desired values for phase margin are between 30 to 60 degrees, and the gain margin was between 2 to 10 dB, which was desirable for closed-loop system design. A system with a significant gain margin and phase margin was stable but may have a sluggish response. On the other hand, a system with a slight gain margin and phase margin may exhibit a more responsive behaviour, but could be prone to oscillations (Kim, 2017).

4. Conclusion

In conclusion, the effect of water temperature on caffeine concentration during brewing was determined. The trend indicates that as water temperature rises, the caffeine concentration also increases. The highest concentration of caffeine was found at 90°C, with 210.58 g/L. Empirical models were developed for coffee brewing using the infusion method at different temperatures. The first-order model with time delay (FOPTD) was fitted to the dynamic process of coffee brewing. The variables of coffee brew at 80°C, 85°C, and 90°C were calculated using estimation (Method 1) and equation method (Method 2). The model at 85°C was simulated into closed-loop systems using a PI controller due to the lower value of RMSE. The controller used had different tuning rules, such as Ziegler-Nichols, Internal Model Control (IMC) and fractional-order controller. The optimized controller depends on its performance and robustness. The best performance was observed with the fractional-order controller using the Chen *et al.* (2008) method, which had the lowest value of Integral of Absolute Error (IAE) at 64.67, lower rise time and settling time, and the best robustness (stability of tuning) as it falls within the desired phase and gain margin.

Conflict of interest

The authors declare no conflict of interest.

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Table 4. PI controller robustness for various tuning rules from Simulink/Matlab.

Tuning Rule	Ziegler-Nichols	Internal Model Control (IMC)	Fractional-Order	
			Chen <i>et al.</i> (2008) method	Gude and Kahoraho method
Gain Margin (dB)/(rad/s)	13.5/0.0706	15/0.0705	11.9/0.0861	9.2/0.0616
Phase Margin (degrees)/(rad/s)	80.5/0.013	82.5/0.0108	52.6/0.0257	43.3/0.025
Close Loop Stability	Stable	Stable	Stable	Stable

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