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Modeling study of coffee extraction at different temperature and grind size conditions to better understand the cold and hot brewing process

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Abstract

In this study, the extraction kinetics, based on total dissolved solid (TDS), at different temperatures (4, 23, 50, and 93°C) for different grind sizes (VMD = 139, 643, 1,450, 1,747 μm) were investigated. Coffee extraction proceeded in initial fast extraction stage followed by a significantly slower extraction stage, which correspond to the extraction from surfaces of broken cells and the extraction from intact coffee cells, respectively. Diffusion inside the coffee particle is a very slow process, so breaking the cells is a very efficient way to increase the mass transfer rate. In addition, the ultimate extraction yield increased with increasing brewing temperature and decreasing of particle size. The Weibull distribution, pseudo-first order and pseudo-second order model were fitted to the kinetics data, with high coefficients of determination (0.687–0.998), and low root mean square error (0.02–0.26%). Meanwhile, exponential equations were created to correlate the derived rate constants ($1/\alpha$, k_1, and k_2) with brewing temperature and particle size to achieve the prediction of brewing extent (TDS_t/TDS_{eqm}) at different temperature-particle size combinations.

Practical applications

This study investigated the kinetics of coffee extraction at different grind size and temperature conditions with the purposes to better understanding the cold and hot coffee brewing process, as well as to predict the coffee extraction. The findings in this study will have practical applications in three folds:

1. Help manufacturers of coffee brew products (ready to drink or concentrate) to better design and control their coffee extraction process.
2. Aid manufacturers of coffee extraction equipment and coffee brewers to improve their products
3. Provide reference information for coffee store, barista, coffee enthusiast, and consumers to brewing a better cup of coffee

1 | INTRODUCTION

Coffee is one of the popular beverages consumed around the world, attributing to its stimulating effect from caffeine, pleasant aroma and flavor, as well as its association with a series of benefits for human health (Higdon & Frei, 2006; Matei, Jaiswal, & Kuhnert, 2012). Typical brewing process extracts soluble solutes, using hot water, from the coffee grounds into the cup. There are many brewing methods, which can be generally categorized into decoction methods (e.g., boiled coffee, Turkish coffee, percolator coffee, vacuum coffee), infusion methods (e.g., filter/drip coffee, Neapolitan coffee) and pressure methods (e.g., French press, moka, espresso) (Clarke &

Vitztbum, 2001; Gloess et al., 2013). Despite the different approaches, the central operation of these methods is the extraction of soluble compounds from the coffee grounds with water, the kinetic of which is affected by variables, in particular grind size, water quality and temperature, brewing time, and brewing ratio (Corrochano, Melrose, Bentley, Fryer, & Bakalis, 2014; Moroney, Lee, O'Brien, Suijver, & Marra, 2015, 2017; Wang, William, Fu, & Lim, 2016).

In general, coffee grounds are considered made up of two fractions: (a) particles of single-cell fragments, also known as fines, of particle size of 25–50 μm; and (b) particles comprising intact coffee cells (cell size in the range of 20–40 μm) (Anderson, Shimoni, Liardon, & Labuza, 2003; Wang et al., 2016). The extraction of coffee solutes from fines and the particle surface is a quick process, involving the direct dissolution/washing of solutes from the cell wall surface. On the other hand, a slower process is expected for the extraction from intact coffee cells, where multiple diffusion mechanisms are involved (Spiro & Selwood, 1984). Diffusion of coffee soluble within the particles is through either cell wall or pores on it (30–50 nm) (Schenker, Handschin, Frey, Perren, & Escher, 2000; Wang & Lim, 2015), with the former being slower than the later. Since higher temperature roasting generates beans with bigger cell wall pores, it is expected that coffee from higher-temperature-short-time process having a faster extraction rate.

Water temperature is another important factor affecting the extraction. Traditional coffee brewing uses hot water (normally > 90°C) as the extraction solvent, but with the introduction and popularity of cold brew, cold water has been increasingly used for coffee brewing (Fuller & Rao, 2017). Temperature affects not only the extraction rate, but also the solubility of the solutes. So, higher temperature normally indicates higher extraction yield at equilibrium. The brewing time required is highly dependent on the brewing temperature and particle size to achieve the optimum extraction yield. For expresso brewing, in which hot water, high pressure and very fine grinds are involved, the extraction only takes about 25–30 s (Andueza et al., 2007; Andueza, Vila, de Pena, & Cid, 2007; Rao, 2008). On the other hand, for cold brewing the extraction can take up to 24 hr to achieve the ideal extraction (Fuller & Rao, 2017). In general, brew ratio [coffee ground: water (w/w)] dictates the strength of the final brew; espresso brew ratio can be as high as 1:1 (Rao, 2008), while drip brewing can be as low as 1:20 (Wang et al., 2016).

Total dissolved solid (TDS) and extraction yield are two important parameters to characterize the brew and brewing process. TDS is often perceived by consumers as "strength," the higher the TDS, the stronger the brew. Extraction yield is defined as the ratio between the mass of the coffee solutes extracted into the cup and the amount of coffee grounds used. As more soluble compounds are being extracted during the brewing process, the extraction yield increases. Low-yield brews are under-extracted and tend to taste flat, while higher-yield brews tend to be "harsh" and "bitter." The ideal extraction yield is 18–22%, as recommended by of Special Coffee Association of America (SCAA). Coffee is composed of over 1800 different chemical compounds and the complex chemistry of coffee makes it challenging to establish definite correlations between the individual chemical constituents and the quality of the final beverage. Therefore, brew strength, extraction yield, along with sensory evaluation are often used as measures of coffee quality.

With the introduction and increased popularity of cold brew over the past decade, coffee's brewing temperature range is now being expanded. To achieve the desired extraction yield, longer brewing time is required than the traditional hot water brewing. In the literature, the brewing times reported for cold brew ranged from 3 to 24 hr (Angeloni et al., 2019; Cordoba, Pataquiva, Osorio, et al., 2019; Fuller & Rao, 2017; Rao & Fuller, 2018; Rao, Fuller, & Grim, 2020). In addition to the brewing temperature, particle size is another important factor that affects the extraction kinetics of coffee. Fuller and Rao's study showed that the brewing time near 7 hr could extract most of the caffeine and 3-CGA for medium and coarse grinds for cold brewing (Fuller & Rao, 2017), but the fine grind was not included in the study which would expect to substantially shorten the time required to achieve the extraction equilibrium. In short, for a specific type of roasted coffee, coffee extraction is a particle size-temperature–time dependent process, which determines the physiochemical and sensory properties of the final brew. Therefore, a comprehensive understanding of those three affecting factors is highly needed, which is currently lacking in the literature.

In this study, the effects of temperature, covering both cold brew and typical hot brew regimes (4–93°C) and grind size of volume mean diameter ranging from 139 to 1747 μm, on the coffee extraction were investigated. Weibull distribution, pseudo-first order and pseudo-second order models were fitted to the extraction kinetics data, with the purpose of: (a) to better understand the cold and hot brewing process; (b) to predict the extraction extent (TDS_t/TDS_{eqm}) based on the grinds size, extraction temperature and extraction time.

2 | MATERIALS AND METHODS

Roasted Columbian coffee beans (*C. Arabica*, medium roast) were supplied by Mother Parkers Tea & Coffee Inc. (Mississauga, ON, Canada).

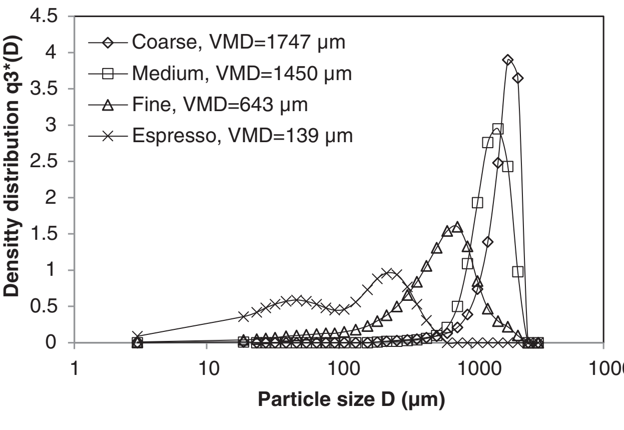

FIGURE 1 Volume particle size distribution of coarse, medium, fine and espresso grind. VMD, volume mean diameter; D, diameter; q3*, volume distribution in logarithmic abscissa

2.1 | Coffee grinding

The roasted coffee beans were grinded in a commercial burr grinder (Bodum® Inc., NY) and then subjected to a series of sieves to narrow down the particle size distribution. Three portions were collected from sieves 1.70–2.38 mm, 0.85–1.70 mm, and <0.85 mm, namely coarse, medium, and fine grinds. Additional size level was achieved by an espresso coffee grinder at 3.3 setting (Mazzer Mini Burr Grinder ETL, Venice, Italy). The particle size distribution of each grind level was analyzed by a particle size analyzer (Helos, Symtech GmbH, Clausthal-Zellerfeld, Germany) and summarized in Figure 1.

2.2 | Coffee extraction, total dissolved solid (TDS) and extraction yield

Three grams of coffee ground (coarse, medium, fine, and espresso) were measured into a 40 mL glass vial containing 36 g of water and then shaken for 10 s to completely wet the coffee ground particles. Extraction was allowed to take place at rest state at 4, 23, 50, and 93°C for a period up to 2,880 min (2 day) or until an extraction equilibrium was achieved. Upon finishing the extraction, the slurry was shaken again before passing it through a filter paper (coarse porosity. Fisherbrand®, Fisher Scientific, Ottawa, Canada) to separate the spent from the brew. The TDS of the brew obtained was measured using the VST Coffee TDS Refractometer (VST Inc.).

2.3 | Extraction kinetics

Weibull distribution model (Equation (1)) (Corzo & Bracho, 2008; Corzo, Bracho, Pereira, & Vasquez, 2008; Cunningham, McMinn, Magee, & Richardson, 2007; Marabi, Livings, Jacobson, & Saguy, 2003; Wang & Lim, 2014), pseudo first- (Equation (2)) and second- (Equation (3)) order kinetic models (Simonin, 2016) were fitted to the extraction kinetics at different temperature and particle size conditions:

$$TDS_t = TDS_{eqm} \times \left[1_{\mathrm{T}}\exp\left[\mathrm{T}\left(\frac{t^{0.5}}{\alpha}\right)^{\beta}\right]\right] \tag{1}$$

$$TDS_t = TDS_{eqm} \times \left[1_{\mathrm{T}}\exp\left(\mathrm{T}t^{0.5} \times k_1\right)\right] \tag{2}$$

$$TDS_t = TDS_{eqm} \times \left[\frac{t^{0.5} \times k_2}{1 + \left(t^{0.5} \times k_2\right)}\right] \tag{3}$$

where t is the extraction time (min); TDS_t (%) is the total dissolved solids of the brew at time t; TDS_{eqm} (%) is the total dissolved solids at equilibrium determined experimentally when the extraction curve reached the plateau; α (min) and β are the scale parameter and shape parameter of Weibull distribution model; k_1 is the rate constant of pseudo-first order (min$^{-0.5}$); k_2 is the rate constant of pseudo-second order (min$^{-0.5}$).

Based on the TDS_{eqm} value, the ideal extraction yield was calculated as:

$$\mathrm{EY}\,(\%) = \frac{TDS_{eqm} \times W_{water}}{W_{coffee}} = \frac{TDS_{eqm}}{brew\ ratio} = TDS_{eqm} \times 12 \tag{4}$$

where W_{water} and W_{coffee} are the weight (36 g) of the water and coffee (3 g) used for brewing, respectively; brew ratio [coffee ground: water, (w/w)] is 1:12.

The effects of temperature on the extraction rate constants were expressed by the following empirical Arrhenius equations (Verbeyst, Oey, van der Plancken, Hendrickx, & van Loey, 2010):

$$k = A \times Exp\left(\frac{-E_a}{RT}\right) \tag{5}$$

Based on the Arrhenius equation, the follow equation was created to describe the effect of particle size on the extraction rate:

$$k = A \times Exp\left(\frac{-L_a}{RT} \times D\right) \tag{6}$$

where E_a is the activation energy (kJ mol^{-1}), which quantify the temperature dependence of k; L_a (kJ mol^{-1} mm^{-1}) is defined to quantify the particle size dependence of k; A is the pre-exponential factor; k is the extraction rate constant at temperature T; R is the universal gas constant (8.314 J mol^{-1} K^{-1}); T is the absolute temperature (K); D is the volume mean diameter of particle (mm).

The combined effects of temperature-particle size on extraction rates (k-value) were modeled using the following exponential equation to achieve the prediction purpose:

$$k = k_0 \times Exp\,(a\mathrm{T}) \times Exp(b\mathrm{D}) \times Exp(\mathrm{cTD}) \tag{7}$$

where T is the extraction temperature (absolute temperature, K); D is volume mean diameter of coffee particles (mm); and parameters k_0, a, b and c are pre-exponential factors, which were estimated from regression analysis.

2.4 | Statistical analysis

The data fitting was conducted using the Solver function of Excel spreadsheet package (Microsoft Corporation, Redmond, WA) by minimizing the total residual sum of squares. The goodness of fit of the model to the data was evaluated by the coefficient of determination (R^2) and mean square error (MSE).

3 | RESULTS AND DISCUSSION

3.1 | Extraction kinetics affected by temperature and grind size

The plots of TDS versus extraction time at 4, 23, 50, 93°C for coffee grounds with different particle sizes are summarized in Figure 2. As

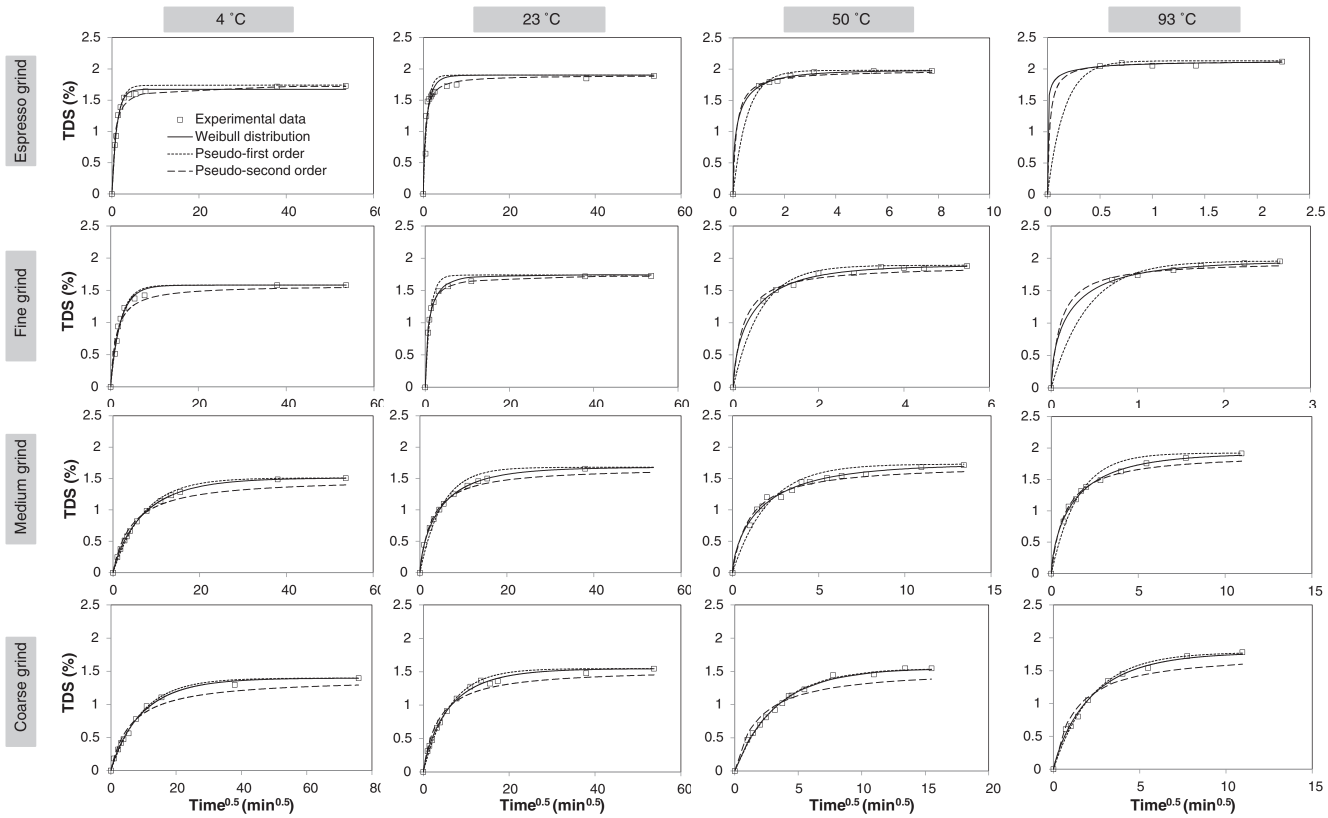

FIGURE 2 Coffee extraction kinetics at temperatures of 4, 23, 50, and 93°C for expresso (VMD = 139 μm), fine (VMD = 643 μm), medium (VMD = 1,450 μm) and coarse grind (VMD = 1747 μm), and model fitting with Weibull distribution (Equation (1)), pseudo-first order (Equation (2)), and pseudo-second order (Equation (3)) models

shown, the extraction process proceeded in two stages; an initial rapid extraction over a short period, followed by a significantly slower extraction stage. The initial fast extraction could be attributed to the rapid solubilization/washing of solutes from the fines and broken cells surfaces, while the slower extraction was due to rate limiting mass transfers (ingress of water and egress of solutes) in the intact coffee cells of larger coffee particles. For the espresso grind, most of the particles are broken cells (Figure 1), and hence the extraction took as short as 15 s to reach equilibrium at 93°C (Figure 2), which is the shortest extraction time within the practical limit of the kinetic experiment in this study. The relative slower extraction for 50, 23 and 4°C should be due to the decreasing dissolution rate with decreasing temperature. In addition, at lower temperature, water has a higher viscosity and surface tension, which slows down the wetting of coffee particles. Generally, extraction for espresso grind was a very quick process; extraction approximate equilibrium in 60 min even for extraction temperature of 4°C.

Figure 2 also shows that the maximum TDS achievable increased from 1.73 to 2.13% (~23% increase) with the increasing of extraction temperature from 4 to 93°C, attributing to the increased solubility of solutes. Higher temperature tends to extract solutes that are otherwise poorly or moderately water-soluble at lower temperatures. The "smooth" taste perceived by consumers for cold brew coffees may indicate that "bitter" and "harsh" compounds are less water soluble in cold temperature (Cordoba et al., 2019; Fuller & Rao, 2017). The "bitter" taste in hot brewed coffee had been attributed to chlorogenic acid lactones and phenylindanes, both of which are derived from chlorogenic acid (Farah & Donangelo, 2006; Frank, Zehentbauer, & Hofmanna, 2006). In addition, some macromolecule compounds and colloid materials, that is, polysaccharides, proteins, melanoidins, and oil, are more soluble or more easily dispersed in hot than cold water, which may explain why cold brews are perceived by consumers having less "body" than hot brew counterparts, due to reduced viscosity. The "body" is described as the sensation of heaviness, richness or thickness, and associated texture by Special Coffee Association of America (SCAA).

Increasing of particle size from espresso to fine grind resulted in a reduction in extraction rate due to presence of more enclosed cells that reduced the mass transfers of water and dissolved solutes. Meanwhile, the maximum solid extracted reduced. For example, at 93°C, the equilibrium TDS for espresso grind and fine grind are 2.13 and 1.96%, respectively, implying that some solutes are not extractable from enclosed cells, such as macromolecular compounds or colloidal materials with lower diffusion rates, thus are remained trapped in the cells. It has been shown that galactomannan and arabinogalactan are the two major polysaccharides present in hot brew coffees, with average molecular weight ranges of 0.2–50 and 0.8–80 kDa, respectively (Arya & Rao, 2007). Since galactomannan is the major contributor of

TABLE 1 Derived model parameters, coefficient of determination (R^2), and root mean square error (RMSE)

Grid size	Temperature (°C)	TDS_{eqm} (%)	Extraction yield (%)	Weibull distribution				Pseudo-first order			Pseudo-second order		
				α ($min^{0.5}$)	β	R^2	RMSE (%)	k_1 ($min^{-0.5}$)	R^2	RMSE (%)	k_2 ($min^{-0.5}$)	R^2	RMSE (%)
Espresso grind	4	1.73	20.76	1.23	0.84	0.972	0.09	0.81	0.913	0.11	1.56	0.876	0.15
	23	1.90	22.68	0.85	0.76	0.982	0.23	1.12	0.887	0.25	2.23	0.894	0.22
	50	1.98	23.58	0.25	0.50	0.990	0.02	1.81	0.968	0.07	7.41	0.981	0.04
	93	2.13	25.44	0.005	0.25	0.996	0.03	6.23	0.968	0.05	44.54	0.995	0.03
Fine grind	4	1.58	18.96	2.22	0.93	0.994	0.11	0.45	0.965	0.11	0.77	0.819	0.18
	23	1.74	20.72	1.17	0.61	0.976	0.07	0.83	0.853	0.15	1.54	0.967	0.05
	50	1.89	22.56	0.51	0.65	0.997	0.04	1.56	0.935	0.09	4.29	0.927	0.10
	93	1.96	23.44	0.25	0.60	0.995	0.02	2.40	0.949	0.06	9.37	0.979	0.05
Medium grind	4	1.51	18.04	7.31	0.87	0.998	0.06	0.14	0.898	0.11	0.23	0.770	0.17
	23	1.68	19.92	5.08	0.72	0.990	0.07	0.20	0.799	0.18	0.36	0.876	0.09
	50	1.73	20.56	1.90	0.69	0.986	0.09	0.49	0.814	0.20	1.00	0.860	0.13
	93	1.92	23.00	1.48	0.69	0.987	0.04	0.66	0.830	0.16	1.26	0.864	0.10
Coarse grind	4	1.40	16.76	9.82	0.92	0.978	0.07	0.10	0.924	0.08	0.16	0.778	0.17
	23	1.51	18.56	6.24	0.84	0.983	0.07	0.16	0.860	0.13	0.28	0.790	0.18
	50	1.54	18.93	3.30	0.95	0.987	0.07	0.30	0.978	0.07	0.55	0.687	0.26
	93	1.78	21.36	2.26	0.89	0.987	0.07	0.45	0.929	0.09	0.80	0.738	0.20

the brew's viscosity, the reduced extraction might result in brew with lower "body" (Arya & Rao, 2007; Navarini et al., 1999). For the medium and coarse grind, the extraction kinetics exhibited more gradual increases in TDS with time, suggesting that the extraction process in these two grinds was mainly governed by the extraction of the solutes from the enclosed cells within the bulk of the particulates, rather than from their surfaces.

Overall, increasing the extraction temperature from 4 to 93°C increased the TDS values at equilibrium by about 23, 24, 27, and 27% for espresso, fine, medium, and coarse grinds, respectively. In comparison, as particle size decreased from 1747 to 139 μm, the TDS values at equilibrium increased by about 24, 22, 19 and 19% when brewing took place at 4, 23, 50 and 93°C, respectively. Thus, it can be concluded that TDS at equilibrium is highly dependent on the extraction temperature and grind size.

3.2 | Model fitting

Weibull distribution, pseudo-first order kinetic, and pseudo-second order kinetic models were fitted to the kinetic data (Figure 2). The estimated parameters and goodness of fit for these models are summarized in Table 1. Weibull distribution model is an empirical model applied to describe various kinetics in food, such as drying and hydration process (Corzo et al., 2008; Corzo & Bracho, 2008; Cunningham et al., 2007). The α parameter is related to the reciprocal of the process's rate constant, representing the time needed to accomplish approximately 63% of the process. β is the shape parameter, related to velocity of the mass transfer at the beginning, the lower the value, the faster the extraction rate at the beginning. When $\beta = 1$, the Weibull distribution model is reduced to first order kinetic equation, while a larger β value (>1) indicates the presence of a lag phase in the mass transfer process. In this study, the derived β values are all smaller than 1, indicating that there was no lag phase during the extraction. The α values decreased with the increasing of extraction temperature and decreasing of grind size, indicating extraction rate increased with the increasing of temperature and decreasing of grind size. On the other hand, the rate constants k_1 and k_2, derived from pseudo first- and second-order kinetics respectively, showed trends in accordance to α parameter with respect to the effects of grind size and temperature. Take k_1 for example, when the extraction temperature increased from 4 to 93°C the rate constant increased from 0.81 to 6.23 min$^{-0.5}$ (8-fold increase) for expresso grind. Moreover, the increasing magnitude of k_1 decreased when increasing particle size to fine (0.45 to 2.40 min$^{-0.5}$; 5.3-fold increase), medium (0.14 to 0.66 min$^{-0.5}$; 4.7-fold increase) and coarse (0.10 to 0.45 min$^{-0.5}$; 4.5-fold increase), implying that the temperature sensitivity of the extraction rate decreased with increasing particle size. Spiro and Selwood (1984) investigated the kinetics of caffeine infusion from coffee and found that rate constants increased about eightfold when increasing the temperature from 25.8 to 84.1°C for particle size range of 850–1,180 μm, which is in agreement with current study.

In general, these three models fitted the experimental data with different degrees of goodness of fit, as reflected by the R^2 values ranging from 0.687 to 0.998 and RMSE ranging from 0.02 to 0.26%. The pseudo-second order kinetic model fitted the medium and coarse grind data with relatively lower R^2 values, ranging from 0.770 to 0.876, and from 0.687 to 0.790, respectively. On the other hand, with two parameters, the Weibull distribution model provided an overall better fit to the extraction data, with the R^2 values ranging from 0.972 to 0.998.

The equilibrium extraction yield was calculated from TDS_{eqm} value based on the assumption that all the water used for extraction was recovered from spent coffee ground (Table 1). For espresso grind, the extraction yield increased from 20.76% at 4°C to 25.44% at 93°C, which is in agreement with previous studies (Angeloni et al., 2019; Wang et al., 2016). In comparison, the extraction yields for the coarse grind were 16.76 and 21.36% at 4 and 93°C, respectively. These observations further demonstrate that the limited mass transport within the coffee ground particles have hindered the extraction process. Reducing the grind size by breaking the cells to increase the surface area is a very efficient way to increase the mass transfer rate and extraction yield (Crossley & Aguilera, 2001; Spiro & Selwood, 1984). Moreover, under the extraction conditions applied, the results suggest that reducing the grind size was more efficient than increasing the temperature to enhancing the extraction rate and yield. As shown in Table 1, the k_1 values for espresso grind at 4°C and coarse grind at 93°C are 0.81 min$^{-0.5}$ and 0.45 min$^{-0.5}$, respectively, indicating the faster extraction rate for the former. Moreover, the extraction yields for these two conditions had comparable values at 20.76% and 21.36% respectively. Other researchers also reported the significance of particle size on extraction yield of other product, such as essential oil extraction from mint leaves (Shrigod, Swami Hulle, Prasad, et al., 2017). However, it is noteworthy that due to the different solubility of the coffee components at different temperatures, along with the limited access of certain compounds in the intact cells, the final compositions of the brew are expected to vary when different temperature–time-grind size conditions are applied. Further compositional and sensory analyses are needed.

3.3 | Effect of temperature and particle size on extraction rate

Since theoretically the extraction rate increased monotonically with increasing temperature and decreasing particle size, the correlations of rate constants derived from the three empirical models with temperature and particles sizes are illustrated in Figure 3 (Peleg, Normand, & Corradini, 2012; Verbeyst et al., 2010). As shown, negative linear correlations were found between ln $(1/\alpha)$, ln (k_1), ln (k_2) and reciprocal of temperature, indicating extraction rate increased with the increasing of extraction temperature. In addition, the absolute slope values increased with decreasing particle size, indicating that coffee with smaller particles had higher activation energy, implying that the extraction rate tended to be more sensitive to temperature

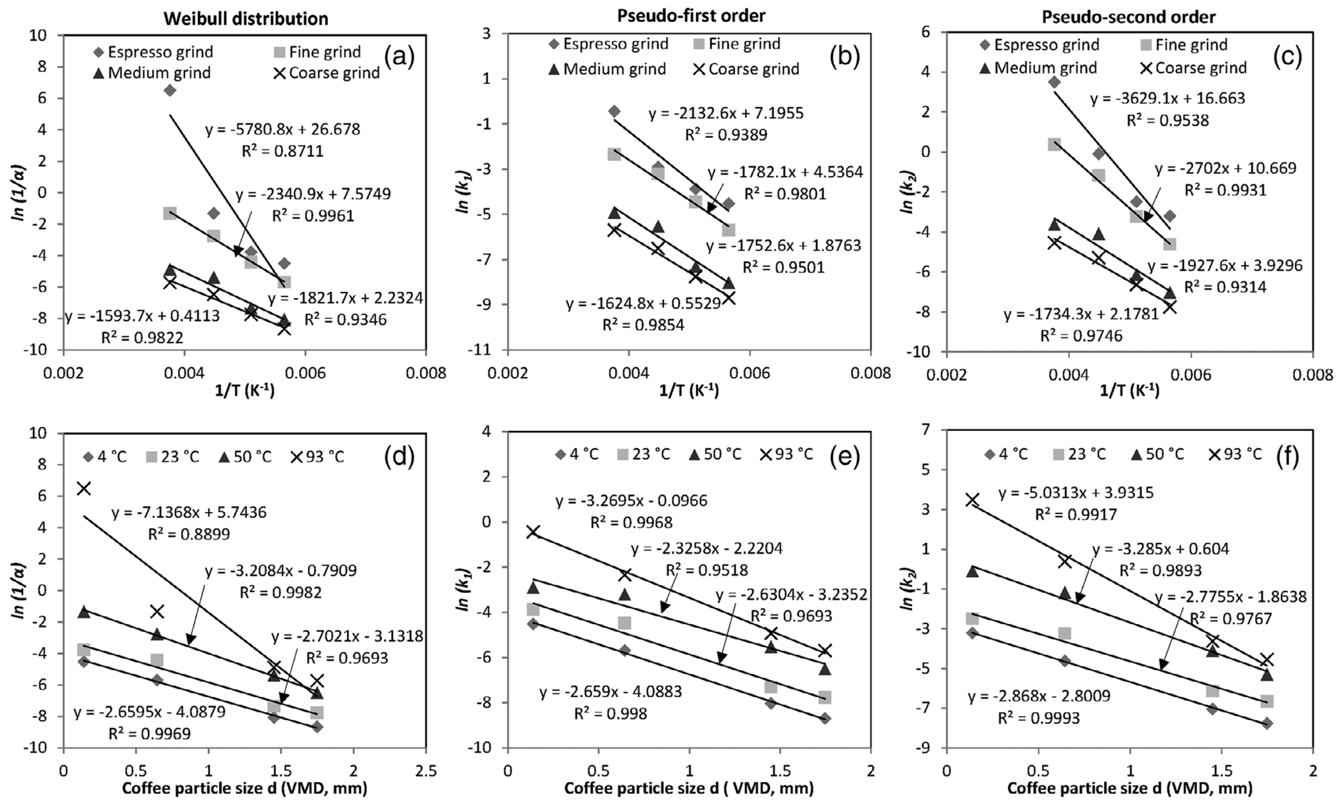

FIGURE 3 Arrhenius plots of rate constants and temperature (a–c), and of rate constants and particle size (d–f)

TABLE 2 Activation energy calculated from the Arrhenius plot between extraction rate and temperature in Figure 3, and derived parameters for the combined temperature-particle size dependence of the extraction rate constants (Equation (7))

Model type	Activation energy (kJ Mol^{-1})				Parameters in Equation (7)			
	Espresso grind	Fine grind	Medium grind	Coarse grind	Ln(k_0)	a	b	R^2
Weibull distribution	48.1	19.5	15.1	13.2	−5.61	0.0214	−1.53	0.94
Pseudo-first order	17.7	14.8	14.6	13.5	−5.17	0.019	−1.36	0.97
Pseudo-second order	30.2	22.5	16.0	14.4	−6.22	0.0261	−1.74	0.94

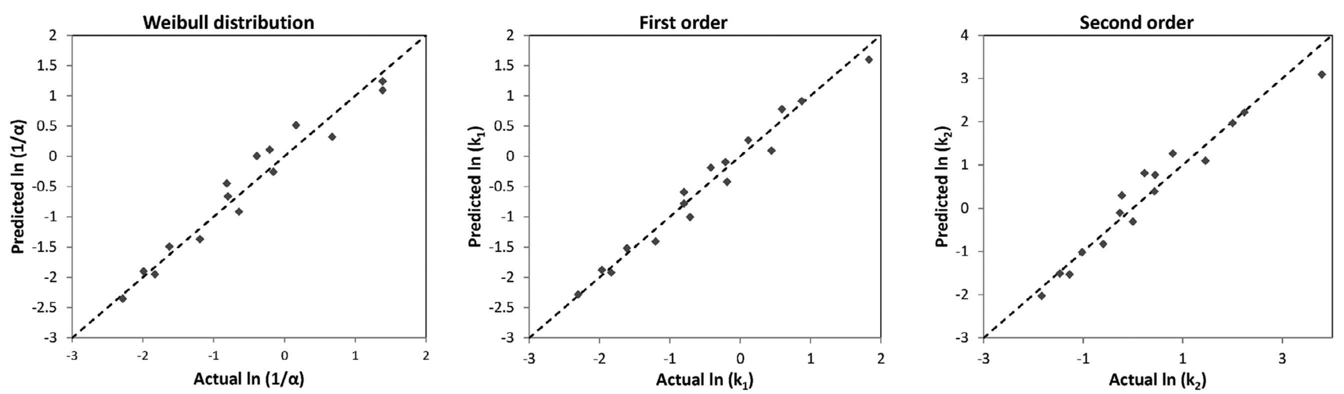

FIGURE 4 Plots between the experimental ln (1/a), ln (k_1) and ln (k_2) values and the values estimated based on the Equation (7)

change as grind size decreased. These phenomena can be explained by the changing of dominant mechanism behind the extraction. For large particles, solutes diffusion within the particle is the rate-determining step, while for fine particles, that is, espresso grind where most of the cells were ruptured, solids dissolution/washing from particle surface is the dominant mechanism which might be more sensitive

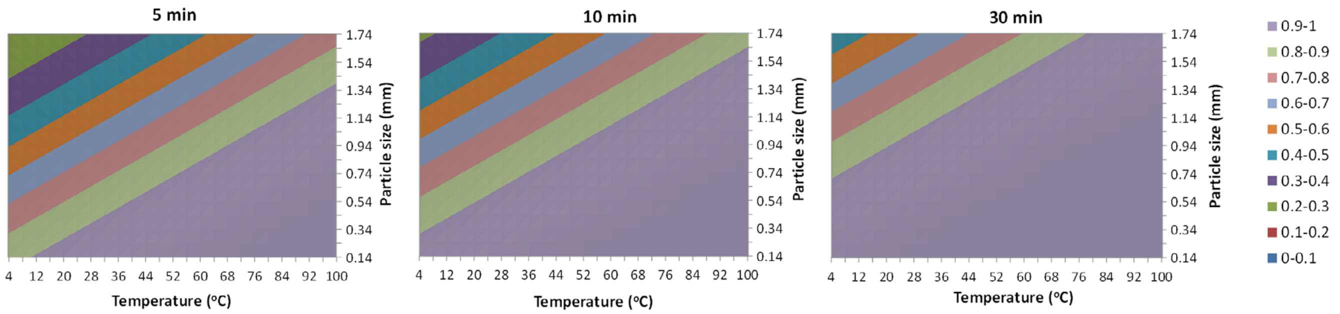

FIGURE 5 Contour plot based on the combination of prediction models Equations (2) and (7), showing the effect of brewing temperature and particle size on the extraction extent (TDS_t/TDS_{eqm}) at 5, 10, and 30 min extraction

to the temperature change. From the slopes of the Arrhenius plots (Figure 3a–c), the activation energy was calculated and summarized in Table 2. Similar pots between natural logarithm of extraction rate and particle size were created (Figure 3d–f), showing strong linear correlations. Figure 3a,d show that the derived rate constant $1/\alpha$ from Weibull model at 93°C for espresso grind is not in a linear relationship with other data points, which could be caused by lack of data points at the beginning of extraction in those conditions. As shown in Figure 2, the extraction of espresso grind at 93°C achieved equilibrium at 0.5 $min^{0.5}$, which was also the minimum time achievable in the current experimental setup. So, the model fittings before 0.5 $min^{0.5}$ were lacking the validation of experimental data, causing three models giving very different extraction rates, of which Weibull distribution model predicted the highest value. Therefore, this data point was deleted before conducting further analysis.

To describe the combined effect of temperature and particle size on the extraction rate constant, linear regression analysis was conducted based on Equation (7). Results showed that the contribution of the interaction term (corresponding to parameter *c*) was not significant ($p > .05$). Therefore, it was deleted, and a reduced model was recalculated. The estimated model parameters ($\ln[k_0]$, *a*, and *b*) are listed in Table 2. The goodness of fit is graphically presented in Figure 4. As shown, all the actual-predicted values data points are randomly fallen on the diagonal lines, indicating a good prediction. Based on the calculated model from Equation (7), the extraction rate constant values can be obtained for different temperature-particle size combinations, and extraction extent (TDS_t/TDS_{eqm}) can be predicted from the kinetics models (Equations (1)–(3)), thus a contour plot can be generated. It should be noted that Weibull model has an additional β parameter, which makes the prediction more complicated. Since pseudo first-order kinetic model has a better fitting to the experimental data than the pseudo second-order counterpart (Table 1), the former was selected to construct the contour plot at extraction time of 5, 10 and 30 min (Figure 5). As shown, at some particle size (<∼1.39 mm)—extraction temperature (>∼10°C) combinations, more than 90% extraction is achievable in 5 min. For example, at hot brewing temperature, for example, 93°C, extraction could achieve 90–100% when the particle size is smaller than ∼1.24 mm, while at cold brewing temperature, for example, 24°C, same extent of extraction can be achieved when the particle size is below ∼0.3 mm. Extraction extent increases with increasing brewing time. At 30 min, coffee extraction at 4°C can reach more than 90% when the particle size is smaller than ∼0.7 mm. In general, Figure 5 dictated the dynamic relationship between particle size, extraction temperature and extraction time, thus will be very useful in directing coffee's cold and hot water brewing process.

3.4 | Conclusions

In summary, this study showed that coffee extraction rate as well as the ultimate extraction yield increased with increasing temperature and decreasing particle size. To achieve specific brew strength and extraction yield, those parameters should be carefully considered. For example, for very fine grind coffee, the brewing time must be minimized if hot water is used to avoid over-extraction, which is how espresso is brewed. But when cold or warm water is used, the extraction time should be extended. In comparison, for coarse grind coffee, where enclosed cells are dominant, extraction is a very slow process even at the hot brewing temperature.

The extraction kinetics of ground coffee at different temperature and particle size conditions were well described by the Weibull distribution, pseudo first-order kinetic and pseudo second-order kinetic models. In addition to temperature, the Arrhenius-like exponential equation could describe the correlation between extraction rate and particle size, making it feasible to predict the extraction at various particle size-temperature–time conditions.

Increasing brewing temperature and decreasing the particle size can help to achieve a higher ultimate extraction yield, but the mechanisms behind are different, thus causing different flavor compounds extracted into the cup. Increasing the brewing temperature generally increase the solubility of all the compounds in coffee, more importantly for those low to medium water soluble compounds, while breaking the cells can help extract more diffusion-limited compounds, specifically macromolecular compounds, that is, polysaccharides, proteins and lipids, which are believed contributing to viscosity and the “body” of the brew. To better understand the effect of particle size-temperature–time on flavor of the coffee brew, further study including sensory evaluation should be conducted.

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AUTHOR CONTRIBUTIONS

Xiuju Wang: Conceptualization; formal analysis; investigation; methodology; validation; writing-original draft. **Loong-Tak Lim:** Funding acquisition; supervision; writing-review & editing.

DATA AVAILABILITY STATEMENT

The data that support the findings of this study are available from the corresponding author upon reasonable request.

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