The Extraction Dynamics and Sensory Quality of Full Immersion Brewed Coffee

By

JIEXIN LIANG
DISSERTATION

Submitted in partial satisfaction of the requirements for the degree of

DOCTOR OF PHILOSOPHY

in

Food Science

in the

OFFICE OF GRADUATE STUDIES

of the

UNIVERSITY OF CALIFORNIA

DAVIS

Approved:

____
William Ristenpart, Chair

____
Jean-Xavier Guinard

____
Tonya Kuhl

Committee in Charge

2023

Table of Contents

List of Figures

List of Tables

Acknowledgements

I am deeply grateful to my major professor, Dr. William Ristenpart, for bringing me on to research when I was a third-year chemical engineering undergraduate. When I discovered my passion in coffee, I am thankful for the opportunity of joining the UC Davis Coffee Center and delve into coffee research. His belief in my potential allowed me to undertake many fascinating studies. I have learned and grown so much in my time here at UC Davis than I imagined. His patience, understanding, guidance, encouragement, and support have been pivotal to my success in this program.

I would like to extend my appreciation to the Specialty Coffee Association for many invaluable opportunities they provided, enabling me to learn and present my work at the Specialty Coffee Expo, Sensory Summit and more. My gratitude goes out to the Coffee Science Foundation for their support of these research projects, with underwriting from Toddy LLC in Chapters 2-6 and Breville Corporation in Chapter 2. I am also thankful to Peet's Coffee for providing me an internship in summer 2019 and their backing in projects in Chapters 2 and 4.

This work would not have been possible without my fellow researchers at the UC Davis Coffee Center. I owe a special thanks to Lik Xian Lim for being the best research partner from the very first day of my coffee research journey. My gratitude extend to Dr. Mackenzie Batali for mentoring me during my first sensory study, and to Juliet Han for expertly roasting the coffees for these projects. Big thanks to my research assistants, Megan Dunkin and Hudson Brown — truly my left and right hands. Additional appreciation goes to Ka Chun Chan, Angela Weber, Sara Yeager, Laudia Anokye-Bempah, Reece Guyon, Andrew Cotter, Jake Dykeman, Diego Docto, and Ashley Thompson for their help and excellent work in coffee research.

While coffee was a significant part of my academic pursuit, my passion for food science extended beyond it. My interest in sensory and consumer science grew tremendously during my PhD studies. I would like to express my gratitude to Dr. Jean-Xavier Guinard for being my sensory mentor and providing me with invaluable guidance and support. Many thanks to the opportunities he gave me to assist in teaching sensory courses, conducting sensory studies, and supporting the exciting project I was so eager to explore. This journey has been deeply rewarding, and I am incredibly thankful for it. I would also like to extend my thanks to the student researchers I collaborated with in Dr. Guinard's lab - Catherine Routt, Keona Kanthatham, and many more - for their assistance in conducting sensory and consumer studies.

I am grateful for my qualifying exam committee: Dr. Julien Delarue, who served as my Chair, Dr. Tonya Kuhl, Dr. Nitin Nitin, Dr. Erin DiCaprio, and Dr. Glen Fox. Their constructive feedback and guidance were instrumental in consolidating my research. I would like to thank my academic advisor, Dr. Glen Fox, for helping me navigate the program. Specifically, I would like to thank to Dr. Tonya Kuhl for her support since my undergrad years and for continuing to serve on my dissertation committee.

I would also love to thank the faculties, scholars, and students in the RMI Sensory Building, who helped me to grow towards a sensory scientist. A special acknowledgment to Dr. Julien Delarue, not just for having me as a TA for his statistics course for sensory science, which I have learned so much through teaching it, but also for encouraging me to apply for an opportunity in Summer 2022, which subsequently laid the foundation for my post-doctoral career. My heartfelt thanks to Dr. Hildegarde Heymann for teaching VEN 215 Sensometrics, the favorite course I have ever taken. It has been both inspiring and life-changing for me in my pursuit of sensory and consumer science. I truly appreciate all the extended discussions and office hours since then. Big thanks to my closest academic friends, Lik Xian Lim, Jane Ong, and Dr. Elena Romeo, for our strong bond and the enriching, inspiring, and memorable times we have shared.

Finally, I would like to express my gratitude to my loved ones outside of academia. To my best friends since middle school, Wenqi Yang, Zixuan Wu, and Yating Li, for growing up with me and sharing all my laughs and tears from overseas. To my dearest friend, Xulun Tan, for being my family in the US. To Kongyun He and Yaqian Feng, for getting every single word I said and sharing feelings I did not express. To Zhaoqi Ren, Xiaolin Yang, and Qinxin Zhao, for all the joyful moments we spent together. To Ziyue Wu for vision, support, and many inspiring conversations. To my dog, Coopa for companionship since 2014 and for always believing I am the best human being on earth.

To Aunt Hong and Uncle Liu, for taking care of me throughout my high school years.

To Dr. Soni Jag and Dr. Mary Chan, for providing such good care for me, allowing me to pursue my goals at a healthier mental and physical condition.

I am grateful for the family I was born in for all the love, care, and enlightenment. To my parents 爸爸妈妈 for giving me this life, raising me with their best, loving every aspect of me, and supporting every single decision I made. To my paternal grandparents 爷爷嫲嫲 for the all precious memories and eternal love. To my maternal grandparents 公公婆婆 for making my favorite foods, and for being my warmest and happiest place in the universe.

To the family I have chosen, Yongjie Huang for staying by my side through the turbulent times in my life, for loving and believing in me unconditionally, for supporting all my goals without hesitation, for dealing with my emotional roller-coaster and helping me through, for cheering me up and experiencing life with me.

Abstract

This dissertation focuses on gaining fundamental understanding of the extraction dynamics and sensory quality of full immersion brewed coffee. The overall goal is to use a diffusion-limited mass transfer model following a “universal brewing curve” to capture and predict the strength, measured in total dissolved solids (*TDS*), and extraction yield, denoted *E*, of full immersion brews under various brewing conditions, and to relate these physical properties (*TDS* and *E*) to sensory properties using sensory descriptive analysis to help achieve desired cup quality of full immersion brewed coffee.

The dissertation is composed of four main stages. First, the equilibrium values of *TDS* and *E* for full immersion brews were investigated over a range of brewing parameters and interpreted using an equilibrium desorption model. The results indicate that the equilibrium *TDS* is approximately inversely proportional to the water/coffee mass brew ratio, while *E* is independent of the brew ratio. Surprisingly, the species-averaged equilibrium constant K was insensitive to grind size, roast level, and hot brew temperature over the range 80-99°C. Furthermore, an analysis of the standard oven-drying method for measuring *E* demonstrated that it yields significant underestimates of the true value at equilibrium, due to retained brew within the spent moist grounds.

The second main stage involves the dynamics of extraction. A diffusion-limited mass transfer model was updated and extended to predict the *TDS* and *E* of full immersion brewed coffee in terms of three parameters: an initial “rinse” concentration (C_0), an equilibrium concentration (C_{eq}), and an effective mass transfer coefficient (k). The model was validated with a series of systematic brewing experiments using various coffee preparation factors, including

varied coffee types, roast levels, brewing temperatures, grind sizes, and agitation rates. The experimental results indicated that (i) increasing brew temperature strongly increases the extraction rate, (ii) light roasted beans extract more quickly than dark roast, and (iii) coffee types from different origins using different post-harvest processing methods yielded no statistically significant differences in extraction kinetics. Furthermore, our agitation experiments demonstrated that occasional and slow manual stirring was as effective as continuous high-speed agitation in terms of increasing the extraction rate, and that the overall extraction rate was primarily limited by diffusion through the interior of the coffee ground.

The third stage involved the impact of coffee ground sedimentation on the dissolved solids concentration in ostensibly quiescent (non-externally agitated) brews. Time-lapse photography observations indicated that dark roasted coffee grounds sediment more slowly than light roasted. Simultaneous measurements of the *TDS* versus both time and vertical position in the brew revealed that full immersion brews undergo a concentration gradient inversion midway through the brewing process. The time scale of the inversion depends sensitively on the roast level of the coffee grounds, which occurs up to a factor of three slower for darker roasts. A key implication is that variations in *TDS* due to different sedimentation rates could possibly confound sensory evaluations of coffees with different roast levels.

Finally, the fourth stage explored the relationship between coffee sensory quality and extraction dynamics of full immersion brewed coffee. A descriptive analysis method was used to explore how the sensory profile of full-immersion brews evolved versus time for different roast levels and brewing temperatures. Our results indicate roast level had the greatest impact on the sensory profile of the coffees, followed by brewing temperature. Surprisingly the effect of brew time, particularly the longer brew time as the TDS approaches equilibrium, had subtler impact than expected at least for the range of brew temperatures and brew time points studied here. The intensity of sweetness was negatively correlated with *TDS*, while 19 other attribute intensities were positively correlated with *TDS*. To increase efficiency, coffee brewing practitioners can reduce brew time beyond equilibrium without changing their products. Interestingly, certain long time cold brews were found to have similar sensory profiles to those of some short time hot brews in light roast, suggesting the potential of achieving similar sensory profiles of long-time cold brews using short-time chilled hot brews through controlled preparation method.

Overall, this dissertation aims to advance the understanding of how coffee preparation factors impact the extraction dynamics, and corresponding *TDS* and *E*, of full immersion brewed coffee, with the ultimate goal of helping coffee practitioners best obtain desired sensory qualities.

Chapter 1. Introduction and literature review

1-1. Importance of coffee quality and opportunities in coffee brewing research

The coffee industry is enormous and is growing continuously around the world. The United States coffee market reached 87-88 billion dollars in 2018 (Specialty Coffee Association, 2019), and 175.6 million 60-kg bags of coffee were consumed globally in 2021-2022 (International Coffee Organization, 2023). The coffee industry can be divided into commodity and specialty, where specialty coffee refers to the high quality coffee produced through meticulous cultivation, processing, roasting, and brewing processes, resulting in flavorful and desirable sensory properties (Hoffmann, 2018; Specialty Coffee Association, 2021; Traore et al., 2018).

The two commercially important coffee species are *Coffea arabica* (Arabica) and *Coffea canephora* (Robusta) (Herrera and Lambot, 2017; Vezzulli et al., 2022). These two coffee species differ in their chemical composition, as Arabica coffee has higher carbohydrates contents, while Robusta has higher caffeine content (Clarke and Macrae, 1987). Arabica coffee is primarily used in the specialty coffee industry because of its unique sensory properties (Hoffmann, 2018). Studies have shown that sensory qualities and personal preference of coffee are the key factors in coffee consumption for consumers (Pinsuwan et al., 2022; Samoggia and Riedel, 2018; van der Merwe and Maree, 2016). Beyond the genetic level of coffee, the complexity of coffee quality arises from numerous influences from the complex production process including planting, harvesting, processing, storing, roasting, and brewing. Variations in these processes lead to differences in the formation of aroma and flavor components in the green coffee bean, roasted coffee bean, and the brew (Pereira et al., 2020). Thus, the sensory quality that can be tasted from a final cup of coffee is not only the result from agricultural, processing, and roasting processes, but it also is significantly affected by the coffee brewing process (Cordoba et al., 2020; Sunarharum et al., 2014).

The coffee brewing process involves extraction of solubles from roasted coffee grounds with water to produce a cup of coffee beverage. The composition of coffee solubles includes polysaccharides, acids, lipids, proteins, oligosaccharides, minerals, caffeine, melanoidins, volatile compounds, and more (Clarke and Macrae, 1987; De Maria et al., 1994; Rufián-Henares and Pastoriza, 2015; Sunarharum et al., 2014; Yeager et al., 2021; Zanoni et al., 1992). The quality of brewed coffee relates to physicochemical characteristics including the total dissolved solids, extraction yield, pH and titratable acidity, and the specific concentrations of non-volatile and volatile compounds (Cordoba et al., 2020; Rao et al., 2020; Sunarharum et al., 2014; Yeager et al., 2021). The total dissolved solids and the extraction yield are by far the most convenient and widely used measurements in relating coffee extraction to quality, both in coffee research and in the coffee industry (Guinard et al., 2023; Lingle, 2011; Lockhart et al., 1957; Mestdagh et al., 2017). The total dissolved solids (*TDS*), also known as strength, is the mass fraction of solubles present in the consumable coffee beverage, and extraction yield (E) is the fraction of solubles removed from the coffee grounds during the extraction with water.

Coffee brewing is intrinsically complex. Different brewing methods with different brewing parameters extracts different solubles, resulting in different cup quality that is typically correlated with *TDS* and *E* (Angeloni et al., 2019a; Cordoba et al., 2020; Gloess et al., 2013). Along with pressurized brewing methods (espresso) and flow-based filtered methods (drip brew or pour-over), full immersions methods (French press, AeroPress, cold brew, cupping) are one of the most commonly used coffee brewing techniques. While the majority of coffee brewing studies have focused on pressurized or flow-based hot water extraction, there is a rising number of full immersion cold brew studies in recent years due to the growing popularity in cold brew consumption (Ahmed et al., 2019; Angeloni et al., 2019b; Batali et al., 2022; Castañeda-Rodríguez et al., 2020; Córdoba et al., 2021; Cordoba et al., 2019; Fuller and Rao, 2017; Mintel, 2017; Portela et al., 2022; Rao et al., 2020; Seninde et al., 2020; The National Coffee Association of USA, 2023; Yeager et al., 2022).

The general process of “full immersion” coffee brewing involves adding a specified quantity of water to a measured mass of coffee grounds placed in a container. The most famous style of full immersion is arguably the French press (Hoffmann, 2018; Wadsworth et al., 2021); yet, there are only a few published research studies on French press brewing specifically (Angeloni et al., 2019a; Gloess et al., 2013; Moroney et al., 2015; Wadsworth et al., 2021). More importantly, the full immersion brewing technique is also utilized in coffee “cupping”, which is a method widely used by coffee industry professionals around the world for quality evaluations. Cupping traditionally involves full immersion using a rigidly prescribed amount of hot water to coffee grounds, with no filtration except pushing the coffee grounds down to the bottom of container, called “breaking the crust”, then skimming off floating coffee grounds with a spoon at a certain time point following the addition of the hot water (Lingle and Menon, 2017). Based on this process, coffee value assessment systems have developed as standard practice in the industry, including for example the Specialty Coffee Association Cupping Protocol (Specialty Coffee Association, 2022) and the Coffee Quality Institute “Q-Graders” certification (Coffee Quality Institute, 2022). Despite the widespread use of cupping procedures for more than a century, there is little scientific justification for the details of this brewing protocol. How these brewing parameters effect the extraction dynamics in brewing process remains unclear, and consequently the consistency and effectiveness of the standard sensory evaluation process in the industry relies on a questionable foundation (Di Donfrancesco et al., 2014; Fioresi et al., 2023; Pereira et al., 2017).

Therefore, to understand the effects of coffee production process and key brewing parameters on the extraction dynamics and subsequent sensory quality of brew, sensory-driven research with a combination of engineering and sensory evaluation approaches are needed to investigate how the physical characteristics of the cup respond to controllable parameters, and how such measurable physical properties (*TDS* and E) relate with the sensory properties of full immersion brewed coffee. For the majority of coffee brewing practitioners and coffee consumers, many practical questions, like what exactly one needs to do to achieve a cup of coffee with desired sensory profile using a full immersion technique, remain to be answered.

1-2. The effects of coffee preparation factors on extraction dynamics

1-2.1 Origins and processing methods

Coffee is produced in regions located near the equator, also known as the “coffee belt”. Regions within this belt have suitable climates, altitudes, and soil conditions for coffee cultivation. Some of the notable coffee-producing countries include Brazil, Colombia, Honduras and Peru in South America, Ethiopia, Kenya, and Uganda in Africa, and Vietnam, Indonesia in Southeast Asia. Within these countries, coffee is produced from smaller regions referred as origins. Different origins have distinct growing conditions including micro-climates, soil composition, and altitudes, which contributes to the chemical composition and flavors of coffee (Bhumiratana et al., 2011; Costa Freitas and Mosca, 1999; Martins et al., 2020; Sualeh et al., 2020). Another crucial factor that contributes to coffee quality is the method of post-harvest processing of removing the pulp and mucilage of coffee cherries through various forms of fermentation and drying to obtain green coffee beans (Lee et al., 2015).

Coffee processing is usually done on or near the farm where the coffee cherries are harvested. Traditional methods of processing include dry processing and wet processing, also known as natural processing and washed processing, respectively. In addition, wet-hulled, honey processing, and other hybrid methods have also emerged (Hoffmann, 2018). Postharvest processing can take from 2 to 4 weeks depending on the procedure (De Bruyn et al., 2017). In dry processing, freshly harvested coffee cherries are laid out for sun drying, where they undergo spontaneous fermentation, and periodically raked by hand to allow air circulation. In wet processing, coffee cherries are depulped mechanically to remove the outer skin and fruit flesh, followed by soaking with water to facilitate fermentation that removes the mucilage layer of the coffee beans. Then, the beans are washed with clean water and dried under the sun. Honey processing is a combination of the processes described above, but instead of water fermentation the depulped coffee beans are laid out on patios or drying beds for sun drying. These three methods above involve a drying step before parchment removal, which is also known as dehulling. In contrast, wet-hulled coffee is only partially dried before hulling, so the seed is fully exposed without the protective parchment while drying (De Bruyn et al., 2017; Elhalis et al., 2023; Hoffmann, 2018; Rotta et al., 2021).

The effects of origin and processing on sensory quality often interplay and are inseparable. For example, washed Ethiopia and honey-processed El Salvador coffees are generally more sour and fruitier than the wet-hulled Sumatra coffee, which is more vegetative and nuttier (Batali et al., 2022). Although coffee flavor and aroma are distinctive from each other depending on their variety, ecological region, and growing conditions, prior studies have shown that the sensory variations via coffee processing method are most likely affected by the composition of flavor precursors in the green beans as a result of fermentation (De Bruyn et al., 2017; Elhalis et al., 2023; Lee et al., 2015; Scholz et al., 2019; Zhang et al., 2019a, 2019b).

Meanwhile, the coffee producing origin and post-harvest processing method have unclear impact on the extraction of solubles in coffee brewing. Prior studies have reported that origin had little effects on *TDS* under consistent brewing protocols, although these coffees were more different in their chemical composition (Batali et al., 2022; Cordoba et al., 2019; Gloess et al., 2014; Yeager et al., 2022). However, these studies solely examined the *TDS* at a single time point during the brewing process. Considering that different processed coffees from different origins have varied chemical composition, a logical presumption arises – different soluble materials extract at different rates. Thus, this question brings research opportunities in investigating how origins and processing methods impact the extraction kinetics in coffee brewing.

1-2.2 Roasting

Coffee roasting is the process of transforming green coffee beans into brown roasted coffee beans. During roasting, the coffee beans undergo complex chemical reactions and changes in physical properties, including many resulting in the flavorful and aromatic characteristics of coffee (Bustos-Vanegas et al., 2018; Nakilcioğlu-Taş and Ötleş, 2019; Wei and Tanokura, 2015). The roast profile of coffee mainly depends on roasting time and temperature, such that the severity of the roast progresses with these two parameters, and the beans become darker in color (Gloess et al., 2014; Schenker et al., 2000; Yeager et al., 2022). Since color is a convenient indicator of roast level, the coffee industry has been using the Agtron Gourmet Scale led by the Specialty Coffee Association to characterize roast level based on color of the roasted beans (Coffee Review, n.d.; Specialty Coffee Association, 2018).

In addition to color change of coffee beans during roasting, other notable changes also occur in their physical properties. Inside the coffee beans, the walls of the porous network are composed of a complex mixture of polysaccharides (Schenker et al., 2000). During roasting, these polysaccharides undergo chemical degradation, and the porous cells expand in volume due to the increasing internal pressure caused by escaping water vapor and CO_2 formation (Redgwell et al., 2002). The cell wall structure loosens as roasting proceeds, so coffee bean density decreases, and porosity increases with roasting temperature (Bustos-Vanegas et al. 2018; Schenker et al. 2000; Ortolá et al. 1998). Generally, the darker the roast, the lower the bean density.

Moreover, the composition of soluble coffee compounds is extremely complex, and coffee roasting contributes largely to the reaction and formation of different flavor and aroma compounds, resulting in different composition of extractable coffee solubles at different roast levels (Rostagno et al., 2015; Rufián-Henares and Pastoriza, 2015; Sunarharum et al., 2014; Tian et al., 2018; Wei and Tanokura, 2015; Yeager et al., 2021). Darker roasts are generally perceived as more burnt, bitter, and roasted, and lighter roasts are generally perceived as more floral, fruity, and sour (Batali et al., 2022). It is well established that a darker roast results in higher pH, lower titratable acidity, and a lower content of chlorogenic acids (Gloess et al., 2014; Yeager et al., 2022, 2021), but the effect of roast level on the total extractable coffee solubles remains unclear. Cordoba et al. found that the impact of roast level on final *TDS* is not significant when the same brewing method and brew temperature are used (Córdoba et al., 2021). Conversely, Gloess et al. and Rao et al. found that roast level did have a significant effect on the total extractable solids, although it is unclear whether these coffee brews had reached equilibrium at the time that the total extractable solids content were measured (Gloess et al., 2014; Rao et al., 2020). Thus, there remains a need to understand the impact of roast level on the extraction dynamics in coffee brewing.

1-2.3 Brewing parameters

Coffee brewing is the final process of extracting soluble compounds from the coffee grounds to produce a flavorful cup of coffee beverage. The major coffee brewing methods include flow-based drip brew or pour-over, pressurized hot water extraction (also known as espresso), and steeping or full immersion brewing that includes French press, cold brew, and cupping. Important coffee brewing parameters include the brew ratio, brew time, temperature, grind size, and pressure (specifically for espresso). Even though the impact of these coffee brewing parameters has been comparatively less studied in full immersion coffee brewing, since, traditional coffee brewing methods such as espresso have traditionally received most of the attention (Cordoba et al., 2020), some overall trends can be drawn regarding the effects of key coffee brewing parameters on soluble extraction regardless of brewing method.

First, the amount of water and coffee grounds added to the brew defines the overall brew ratio. Lower water/coffee brew ratio increases the total dissolved solids content in the brew, while the extraction yield from the grounds depends sensitively on other brewing parameters such as brewing time and grind size (Andueza et al., 2007; Batali et al., 2020b; Lingle, 2011; Lockhart et al., 1957). Regarding brewing temperature, the general effect is also straightforward. Studies have shown consistently that increasing brewing temperature results in higher brew strength and extraction, in accord with the general observation that soluble compound solubility increases with temperature (Andueza et al., 2003b; Mestdagh et al., 2017; Rao et al., 2020; Voilley and Simatos, 1979; Wang and Lim, 2021). Similarly, longer extraction time also increases extraction yield and the accumulated extractable contents in the brew as the contact time between water and coffee grounds increases (Batali et al., 2020a; Melrose et al., 2018; Moroney et al., 2015; Zanoni et al., 1992). The particle size of coffee grounds also plays an important role in determining the coffee extraction. Grinding roasted coffee beans promotes the release of coffee aroma compounds from coffee preparation process to brewing (Akiyama et al., 2003;

Bhumiratana et al., 2011), and it further facilitates extraction of soluble materials by increasing the surface area with smaller grind sizes. Studies have shown that the both total dissolved solids and extraction yield increases with decreasing particle size (Andueza et al., 2003a; Cameron et al., 2020; Cordoba et al., 2019; Moroney et al., 2015; Severini et al., 2015; Voilley and Simatos, 1979; Wang and Lim, 2021).

Although the above-mentioned general trends are well established, the precise relationship between these brewing parameters and *TDS* and *E* remains unclear. Given the importance of *TDS* and *E* as measures of extraction dynamics and the subsequent sensory quality of brewed coffee, a crucial question is: how can we predict *TDS* and *E* versus brew time in terms of controllable brewing parameters, such as the brew ratio, brewing temperature, and grind size? Because the extraction process depends highly on the precise brewing methods, several groups have worked on developing theoretical models to predict the brew strength and extraction yield on pressurized or flow extractions (Cameron et al., 2020; Corrochano et al., 2015; Fasano and Talamucci, 2000; Melrose et al., 2018; Moroney et al., 2015). Comparatively less theoretical work has focused on extraction dynamics of soluble substances in full immersion brews in the context of practical application within the coffee industry (Moroney et al., 2016; Voilley and Simatos, 1979; Wang and Lim, 2021; Zanoni et al., 1992). Thus, a simple, universal, and practical model to capture, compare, and predict the extraction dynamics in full immersion brewed coffee in response to coffee preparation factors is desirable.

1-3. The connection between extraction dynamics and sensory quality

To date, it is well-established that the sensory quality of brewed coffee, relying on sensory properties and consumer hedonic response, is highly associated with *TDS* and *E* (Batali et al., 2020b; Cotter et al., 2021; Frost et al., 2020; Guinard et al., 2023; Lockhart et al., 1957). Notably, the scientific exploration of these key metrics for coffee cup quality started since the mid-20th century. Dr. Ernest E. Lockhart from the Coffee Brewing Institute was the first to relate coffee cup quality to the total solids and extraction yield in brewed coffee. This early works suggested that there is a range of *TDS* (1.15% - 1.35%) and *E* (18% - 22%) that yields the “ideal” coffee for optimal sensory quality and consumer acceptance (Lockhart et al., 1957). The concept was compiled into the classic Coffee Brewing Control Chart, as discussed at length in the Coffee Brewing Handbook published by the Specialty Coffee Association. This chart has served as the basis for educational and training purposes in the coffee industry since then (Lingle, 2011).

These early results have been updated and expanded using modern sensory methodologies to better capture the broad range of flavors possible in brewed coffee (Batali et al., 2020b; Frost et al., 2020, 2019; Guinard et al., 2023). In particular, the new Coffee Brewing Control Chart revealed that bitter and roasted attributes are strongly associated with high *TDS* and E; acid/sour, citrus, and berry attributes are associated with high *TDS* and low E; black tea notes are maximized in the low *TDS* and high *E* region, and the perceived “sweet” flavor impression is maximized at low *TDS* and low *E* (Guinard et al., 2023). These differences in *TDS* and *E* also drive consumer preference of the same roasted coffee brewed to different sensory attributes (Cotter et al., 2021).

Furthermore, detailed sensory analysis brought novel understandings of *TDS* and *E* in drip brewed coffee to the coffee industry. Systematic sensory and consumer study has shown that both grind size and basket geometry under the same brewing protocol yield significantly different *TDS*, which impact the sensory quality and consumer acceptance of drip brewed coffee (Frost et al., 2019). In relating *TDS* with sensory attribute intensities in brewed coffee, it was found that as *TDS* decreases, bitter, sour, and smoky/burnt flavor also decrease, but sweet and tea/floral flavor increase (Batali et al., 2020a). Furthermore, the sensory properties of brewed coffee were found to be governed primarily by differences in *TDS* and *E* instead of brewing temperature; Batali et al. showed that hot brewing temperature from 87 to 93°C, at fixed *TDS* and E, had little impact on the sensory profiles of drip brew coffee (Batali et al., 2020b). More importantly, sensory analysis showed that a considerable amount of sensory attributes varied significantly across different regimes of the classic Coffee Brewing Control Chart, indicating the sensory properties of coffee brewed to different combinations of *TDS* and *E* are far beyond simple characteristics summarized as “underdeveloped”, “bitter”, “ideal”, “weak” or “strong” (Frost et al., 2020).

These recent findings are shifting the understanding of coffee quality from a one-size-fit-all “ideal” belief to a more consumer-centric concept in bringing different desirable sensory profiles to different consumers. Accordingly, the industry needs improved understanding of how coffee extraction dynamics yield desirable values of *TDS* and E. A key point is that these aforementioned sensory and consumer studies only focused on drip brew coffee. There remain unaddressed research opportunities regarding the extraction dynamics and sensory quality of an equally important brewing technique, full immersion coffee brewing.

1-4. Objectives and hypotheses

The research in this dissertation focuses on gaining fundamental understanding of the extraction dynamics and sensory quality of full immersion brewed coffee in response to coffee preparation parameters, from bean to cup. The overarching goal is to use a diffusion-limited mass transfer model to predict the *TDS* and E, and to subsequently gain control in the cup quality by relating the physical properties to the sensory properties of full immersion brewed coffee.

The specific objectives of the research are as follows. The first aim is to measure and predict the strength and extraction yield of full immersion brewed coffee versus extraction time for varied origin, roast level, brew ratio, grind size, brew temperature, and agitation rate. The second aim is to investigate the roles of coffee ground sedimentation in governing the extraction dynamics in ostensibly “unagitated” full immersion brews. Then, the third aim is to relate the physical properties (*TDS* and E) to the sensory properties of the full immersion coffee over time at various brewing temperatures and roast levels.

The central hypothesis of the research is that the dynamic *TDS* and extraction of full immersion brews over a wide range of coffee brewing parameters (e.g., grind size, brew ratio, water temperature, agitation) can be captured using an updated and extended diffusion-limited mass transfer model. Likewise, the sensory quality of full immersion brewed coffee for a wide range of roast levels can be quantified and controlled using the model with combination of descriptive analysis. These three objectives and the overall hypothesis were explored through following four main stages of the investigations.

In the first stage (Chapter 2), an adsorption-desorption model was developed to capture and predict the equilibrium *TDS* and *E* of full immersion coffee brewed at various hot brewing temperatures (80-99°C), five different grind sizes, and five different roast levels.

In the second stage (Chapter 3), a diffusion-limited model was updated and extended for the extraction dynamics of full immersion brewed coffee. This model was validated with experimental data from a massive investigation on the effects of roast level (Light, Medium, Dark), brewing temperature (4°C, 22°C, 94°C), and post-harvest processing method from different origins (El Salvador – washed, Ethiopia – honey processed, Sumatra – wet hulled), on the extraction dynamics of full immersion brewed coffee, comprising 3,420 individual measurements. The diffusion-limited model is further studied in Chapter 4, which explores the impact of agitation rate and elucidates the effects of coffee grind size, agitation rate, and their interplay effects on the extraction dynamics. Systematic brewing experiments studied coffees brewed at 99°C with 7 different grind size settings range from 360 to 1319 µm, continuous agitation with magnetic stirrer at various agitation rates, and interval agitation with a spoon.

In the third stage (Chapter 5), the concentration (*TDS*) gradient in ostensibly quiescent, non-externally agitated full immersion brews and the corresponding rate of coffee grounds sedimentation versus time at different roast levels was studied. The goal was to understand the impacts of the transient sedimentation process and roast level on the concentration profile of *TDS* within the brew, and their subsequent impacts in the sensory evaluation process using full immersion methods.

Finally in the fourth stage (Chapter 6), the extraction dynamics were related to the sensory quality with a sensory-driven engineering research process. A generic descriptive analysis method coupled with systematic physicochemical measurements was used to explore the flavor profiles and investigate the drivers in sensory quality of full immersion brewed coffee over time at various roast levels (Light and Dark), brewing temperatures (4°C, 22°C, 92°C).

Chapter 7 summarizes main results and explores remaining unanswered questions that could be addressed in future work. Overall, with systematic brewing experiments and detailed sensory analysis, this dissertation aims to contribute to the growing field of coffee brewing research and to open new brewing avenues for continuous improvement in the coffee industry.

Chapter 2. An equilibrium desorption model for the strength and extraction yield of full immersion brewed coffee

Note: this chapter was based on published materials in *Scientific Reports*

Liang, J., Chan, K.C. & Ristenpart, W.D. An equilibrium desorption model for the strength and extraction yield of full immersion brewed coffee. *Sci Rep* **11**, 6904 (2021). https://doi.org/10.1038/s41598-021-85787-1

Author contributions:

J.L. co-designed the study, conducted experiments, performed data analysis and figure preparation, and co-wrote the published manuscript. K.C.C. conducted experiments. W.D.R. secured funding, co-designed the study, advised data analysis and co-wrote the published manuscript.

In addition, the authors would like to acknowledge Joanne Yang at Peet's Coffee for performing the particle grind size measurements.

2-1. Abstract

The sensory qualities of brewed coffee are known to be strongly correlated with the total dissolved solids (*TDS*) and extraction yield (*E*) of the brew. Here, we derive a predictive model for the *TDS* and *E* of full immersion brewed coffee using a pseudo-equilibrium desorption approach. Assuming a single, species-averaged equilibrium constant K yields theoretical predictions indicating that the *TDS* is approximately inversely proportional to the water/coffee mass brew ratio, while *E* is independent of the brew ratio. Our experimental results strongly accord with both theoretical predictions, and indicate that *E* is approximately 21% over a wide range of brew ratios. An analysis of the standard oven-drying method for measuring *E* indicates that it yields significant underestimates of the true value at equilibrium, due to retained brew within the spent moist grounds. We further demonstrate that K is insensitive to grind size, roast level, and brew temperature over the range 80-99°C. Taken together, our results indicate that full immersion brewing offers precise control over the *TDS* at equilibrium but little control over *E*, and that practitioners should pay careful attention to their brew ratio as the most important parameter for full-immersion brewing.

2-2. Introduction

The immense popularity of coffee beverage is driven in part by its complex sensory profile(Harwood et al., 2020; Samoggia and Riedel, 2018; Spencer et al., 2016), which in turn is due to its complicated chemical composition: brewed coffee contains several hundred different species that are known to affect the sensory profile(Sunarharum et al., 2014), the concentrations of which can be modified by choice of brewing technique(Cordoba et al., 2020; Gloess et al., 2013). Because of this complexity, many investigators and coffee industry practitioners focus not on the specific chemical composition, but instead quantify the mass concentration of all dissolved species in the beverage. This quantity, also known as the “brew strength,” is often characterized as the “total dissolved solids” (*TDS*), and can be related by mass conservation arguments(Ristenpart and Kuhl, 2017) to the extraction yield *E* from the solid coffee grounds (sometimes also known as the percent extraction, PE). Early work by Lockhart established that the *TDS* and *E* are good indicators for the quality of coffee, with *TDS* values near 1.25% and *E* values near 20% identified as “ideal.”(Lockhart et al., 1957) These early results have more recently been updated and expanded with modern sensory methodologies to better capture the broad range of flavors possible in brewed coffee(Batali et al., 2020b; Frost et al., 2020). In particular, systematic experiments showed that higher *TDS* is strongly associated with increased bitterness, smoky, and roast-like aromas; higher *TDS* and low *E* is associated with higher sourness and citrus; while lower *TDS* is associated with increased sweetness and tea-like/floral at low or high *E* respectively. These differences in sensory attributes help drive consumer preference of the same roasted coffee brewed to different strengths and extraction yields (Cotter et al., 2021).

Given the importance of *TDS* and *E* in the sensory profile of brewed coffee, a natural question is: how do we predict these quantities in terms of brewing control parameters, like the brew ratio, brewing temperature, water flowrate, and coffee grind size? Towards that end, several groups have examined theoretical models aimed at predicting the brew strength and extraction yield. Fasano and Talamucci presented mathematical models primarily focused on describing the mass transport phenomena taking place in an espresso machine (Fasano and Talamucci, 2000). Moroney and colleagues used multiscale methods to characterize the spatial-temporal dynamics of coffee extraction by hot water from a fixed coffee bed (Moroney et al., 2015), and subsequently developed a model reduction of this work to describe coffee extraction kinetics in a well-mixed system (Moroney et al., 2016). They further compared one-dimensional flow models to computational fluid dynamics modelling for packed bed coffee extraction (Moroney et al., 2019). Melrose et al. introduced a simpler "base model" for coffee brewing through a packed bed of coffee grains to generate *TDS* and extraction yields versus brew parameters (Melrose et al., 2018). Most recently, Cameron et al. developed a detailed model for espresso extraction with the assumption of homogeneous flow through the coffee bed, yielding predictions for how to increase the extraction yield (Cameron et al., 2020).

Notably, almost all of the above theoretical work focused on flow extractions, where fresh water flows into the grounds and then extracted brew flows out the other side. Another equally important class of brewing technique, however, involves "full immersion" brewing. Also known as "steeping," this method involves immediate addition of all of the water to the coffee grounds, and then waiting for the extraction to proceed before finally removing the coffee grounds. A classic example is the well-known "French press" style of brewer, but other brewer types such as

Toddy-style cold brewers or Japanese vacuum brews also involve full immersion. A particularly important type of full immersion brewing is “cupping,” which is the traditional method that coffee industry professionals around the world use to assess the quality of different coffee lots (Feria-Morales, 2002; Lingle and Menon, 2017). Cupping traditionally involves full immersion of a rigidly prescribed amount of hot water to coffee grounds, with no filtration except skimming off floating coffee grounds with a spoon at a certain time point following the addition of the hot water (Specialty Coffee Association, n.d.).

Despite the widespread popularity of full immersion brewing methods, relatively little theoretical work has examined it. Moroney et al. used their multiscale flow extraction model to investigate the limiting case of batch-wise brewing (Moroney et al., 2016, 2015); they solved the resulting set of coupled differential equations numerically and via matched asymptotic expansions to assess *TDS* versus time. This approach, however, required multiple fitting parameters, and to date several key questions about full immersion brewing remain unanswered. For example, how does the brew ratio affect the strength of full-immersion coffee? How does it affect the extraction yield? What is the impact of the brew temperature, grind size, and roast level on these quantities?

Here, we develop a theoretical model for full-immersion brewing of coffee to answer these questions. We assume the beverage solution and solid coffee grounds reach an effective equilibrium between desorption and adsorption that can be approximated with a single equilibrium constant reflecting the average behavior of all chemical species present. The resulting model predicts that the brew strength varies approximately inversely with brew ratio, but that the extraction yield at equilibrium is independent of the brew ratio. The model further predicts that retained liquid following filtration will yield artificially low measurements for the extraction measured via the standard oven drying approach. Experimental measurements accord with these model predictions, and further indicate that the effective equilibrium constant is insensitive to roast level, grind size, and brew temperature at least over the range of 80 to 99 °C. The results presented here provide insight on how full immersion brewing techniques can be optimized to yield desired brew strength that may yield desired sensory profiles (Cotter et al., 2021).

2-3. Theory

2-3.1 Definition sketch for full immersion brewing

The main goal of this section is to derive theoretical predictions for the *TDS* and *E* of full immersion brew, focusing on the brewing and characterization process depicted schematically in Fig. 2-1 and using nomenclature summarized in Table 2-S1. Our approach is based on well established principles in chemical engineering (Fogler, 2020), but which to our knowledge have not been used in the context of coffee. Initially, a known mass of coffee grounds (M_g) and a known mass of hot water (M_w) is added to the brewer. The ratio of these masses is defined as the brew ratio,

$$R_{brew} = \frac{M_w}{M_g}. \tag{2-1}$$

Upon addition of the water to the coffee grounds, mass transfer proceeds and the *TDS* of the liquid increases and eventually plateaus to a steady value (behavior that is readily verified experimentally, as discussed below). We neglect the potentially complicated dynamics that occur during the transient phase to focus on the final 'equilibrium' brew strength of the liquid. This condition is not a true thermodynamic equilibrium since the brewed coffee can continue to undergo subtle changes (such as evaporation of volatiles or gradual acidification due to slow chemical reactions), but for the time scales of interest (measured in minutes or tens of minutes) we assume the system achieves an effective pseudo-equilibrium.

After the brew strength reaches a final steady value, the brew is then filtered, yielding a mass of beverage M_{brew} that could be consumed, and leaving behind a mass M_{spent} of spent moist coffee grounds. Finally, a standard procedure to measure the overall extraction of the brew is to place the spent moist grounds in an oven to bake off the water and measure the residual mass. As discussed in detail below, M_{spent} contains both the unextracted coffee grounds plus some retained beverage that contains part of the dissolved coffee species, complicating interpretation of the measured extraction yield via oven drying.

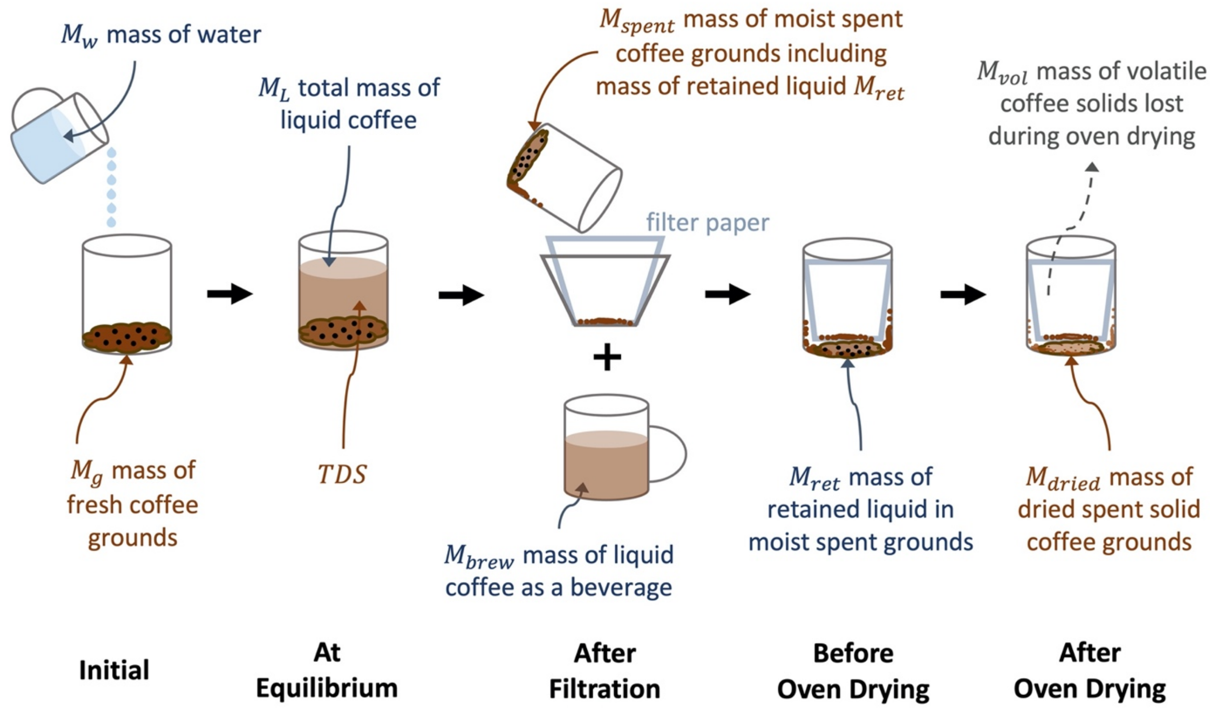


Figure 2-1. Schematic of a full immersion brew with subsequent oven-drying measurement of extraction.

2-3.2 Equilibrium Desorption Model

We focus first on a prediction for the equilibrium *TDS*. Ground coffee contains hundreds of individual chemical species, all of which have a unique solubility: some species are highly soluble and will completely dissolve, while others are weakly soluble and will hardly dissolve. Instead of tracking individual species, we assume that the overall behavior can be described by a single, average equilibrium constant with corresponding rates of desorption and adsorption from and onto the solid insoluble coffee ground matrix. Specifically, these rates are related as

$$C_A \underset{k_A}{\overset{k_D}{\rightleftharpoons}} C_D \,, \tag{2-2}$$

where C_A is the mass concentration of adsorbed soluble coffee species, C_D is the mass concentration of dissolved soluble coffee species, k_D is the first order rate constant of desorption, and k_A is the first order rate constant of adsorption. For simplicity in relating theory to experimental observations, both mass concentrations are per unit mass of liquid, M_L, such that

$$C_A = \frac{M_A}{M_L}, \tag{2-3a}$$

$$C_D = \frac{M_D}{M_L}. \tag{2-3b}$$

By this definition, C_D is equivalent to the *TDS*. We assume here that volatilization of the coffee solids is negligible, so the soluble coffee species are either dissolved in solution in liquid phase, or adsorbed on the solid coffee grounds. Accordingly, the total mass of soluble species is conserved,

$$M_A + M_D = M_{tot} \tag{2-3}$$

where M_{tot} is the total mass of extractable coffee species (and $C_{tot} = M_{tot}/M_L$ is the total concentration). This quantity can be expressed in terms of the maximum extraction yield possible in the coffee,

$$M_{tot} = E_{max} M_g, \tag{2-4}$$

where E_{max} is the maximum extraction of coffee grounds. Typically E_{max} is observed to be around 0.3, that is, only about one third of the mass of roasted coffee is soluble in water (Moroney et al., 2015).

After the initial complicated dynamics that occur when the water is added to the coffee grounds, the brew eventually reaches equilibrium such that the concentrations reach a steady state,

$$\frac{dC_A}{dt} = 0 = -k_D C_A + k_A C_D, \quad (2\text{-}5)$$

which with equation (2-3) yields

$$C_D = \left(\frac{k_D}{k_D + k_A}\right) C_{tot} \ . \quad (2\text{-}6)$$

We define the equilibrium constant,

$$K = \left(\frac{k_D}{k_D + k_A}\right) . \quad (2\text{-}7)$$

and substitution of equation (2-4) yields

$$C_D = K E_{max} \frac{M_g}{M_L} . \quad (2\text{-}8)$$

Note that M_L is not known a priori but it is readily related to the mass of water added and the mass of dissolved coffee species present in the brew,

$$M_L = M_w + M_d. \quad (2\text{-}9)$$

This formulation assumes that any water mass lost to evaporation, or water mass lost to physical adsorption onto the solid coffee grounds, is negligible. Substitution of (9) into (8), recalling equation (2-1), and rearrangement yields the equilibrium *TDS*,

$$C_D = TDS = \frac{K E_{max}}{R_{brew} + K E_{max}} . \quad (2\text{-}10)$$

Under typical conditions, R_{brew} is on the order of 5 to 25, while E_{max} is approximately 0.3. Thus, if K is order one or smaller, then to good approximation the second term in the denominator is negligible and we have the simplified expression

$$TDS = \frac{K E_{max}}{R_{brew}} . \quad (2\text{-}11)$$

2-3.3 Extraction Yield at Equilibrium

Given the preceding analysis, the corresponding extraction yield at equilibrium is readily derived. By definition, the extraction yield *E* is the mass of solid coffee that dissolves into the liquid phase per original mass of coffee grounds,

$$E = \frac{M_d}{M_g}. \quad (2\text{-}12)$$

By equations (2-3b) and (2-8), we have

$$M_d = C_D M_L = K E_{max} M_g, \quad (2\text{-}13)$$

and substitution back into equation (2-12) yields the final result,

$$E = K E_{max}. \quad (2\text{-}14)$$

We emphasize that equation (2-14) is the theoretical prediction for the actual extraction yield of the brew at equilibrium, not after drying spent grounds in the oven. Notably, E is predicted to be completely independent of the brew ratio, and to depend only on the equilibrium constant and the maximum extraction. In other words, the brewer can arbitrarily vary the strength of the brew as per equation (2-11) simply by altering the brew ratio, but the extraction yield at equilibrium is adjustable only by altering the ingredients: in principle, both K and E_{max} could depend on the composition of the coffee, the composition of the water, and the system temperature.

A key point is that the extraction yield at equilibrium cannot be measured directly, but we can relate it to the *TDS* using mass conservation arguments. Specifically, from equations (2-3b) and (9) the mass of dissolved solids is related to the *TDS* as,

$$M_d = \frac{TDS}{1-TDS} M_w, \quad (2\text{-}15)$$

and substitution into equation (2-12) yields

$$E = \frac{TDS}{1-TDS} R_{brew}. \tag{2-16}$$

It is straightforward to verify that substitution of equation (2-10) into equation (2-16) yields $E = KE_{max}$, i.e., expressions (2-14) and (2-16) are self-consistent. Because the *TDS* is readily measured experimentally, equation (2-16) provides an easy means to assess the extraction yield of a full-immersion brewed coffee.

2-3.4 Extraction Yield from the Oven Drying Method

Finally, we consider a theoretical prediction for extraction yield when measured experimentally using the oven drying method. In this technique, the brewed liquid is filtered from the spent grounds, and the spent moist coffee grounds are dried in an oven to remove all the water (Fig. 2-1). The extraction yield can then be calculated using the difference of coffee grounds before brewing and after drying,

$$E_{oven} = \frac{M_g - M_{dried}}{M_g}, \tag{2-17}$$

where M_{dried} is the experimentally measured mass of dried spent grounds. Note that $E \neq E_{oven}$ because they measure different quantities: E reflects the amount of dissolved coffee at equilibrium in the beverage, while E_{oven} reflects all solids left behind after filtration and baking. In particular, the spent moist grounds invariably include some retained brew with dissolved solids that must be accounted for, and baking the grounds for several hours can cause some fraction of the mass to volatilize and escape into the gas phase. By conservation of mass, the mass of dried grounds must equal the original mass of coffee grounds minus what was removed by brewing and baking,

$$M_{dried} = M_g - TDS \cdot M_{brew} - M_{vol}. \tag{2-18}$$

Here M_{brew} is the mass of brewed coffee delivered into a separate container following filtration, while M_{vol} is the mass of coffee solids volatilized while baking in the oven. Note that M_{brew} depends on how effectively one pours off the brew (i.e., one can leave behind a little or a lot of liquid amongst the spent grounds), but in any case M_{brew} is readily measured. Substitution of (18) into (17) yields

$$E_{oven} = TDS\,\frac{M_{brew}}{M_g} + \frac{M_{vol}}{M_g}. \tag{2-19}$$

If we define M_{ret} as the mass of liquid retained within the spent moist grounds following filtration, then

$$M_{brew} = M_L - M_{ret}, \tag{2-20}$$

and substitution of equations (2-8) and (2-14) yields

$$E_{oven} = KE_{max}\left(1 - \frac{R_{ret}}{R_{brew}+KE_{max}}\right) + R_{vol}. \tag{2-21}$$

Here $R_{ret} = M_{ret}/M_g$ is the liquid retention ratio during filtration and $R_{vol} = M_{vol}/M_g$ is the volatilization ratio during baking. If the latter quantity is negligible, and for brew ratios such that $R_{brew} \gg KE_{max}$, then to good approximation we have

$$E_{oven} = KE_{max}\left(1 - \frac{R_{ret}}{R_{brew}}\right). \tag{2-22}$$

In other words, the extraction yield as measured via oven drying will invariably be smaller than the true extraction yield at equilibrium, with the magnitude of the discrepancy decreasing as the brew ratio increases. The retention ratio depends on how efficiently one pours off the brew, but to calculate it, substitution of (2-9) and (2-15) into (2-20) and rearrangement yields

$$R_{ret} = \frac{R_{brew}}{1-TDS} - \frac{M_{brew}}{M_g}. \tag{2-23}$$

All of the terms on the right-hand side of equation (2-23) are readily measured experimentally.

2-4. Experimental Methodology

The main goal of the experimental work was to assess the validity of equations (2-10), (2-14), and (2-21) for the equilibrium *TDS*, E, and E_{oven} respectively. Two separate suites of experiments were performed. First, a single type of coffee was tested systematically in 1-liter full immersion brews, using the methodology presented in Fig. 2-1, for a wide variety of brew ratios, brew temperatures, and grind sizes. Second, because the traditional cupping method is used so ubiquitously in the coffee industry, we tested five different coffees at different roast levels with the cupping method over a wide range of brew ratios. Specific brewing parameters for each brewing experiment are summarized in Table 2-1.

Experiment	**Brew Temperature (°C)**	**Brew Time (minutes)**	**Brew Ratio**	**Grind Size Setting***	**Distinct Roasts**	**Trial Replicates**	**Total Number of Brews**
3.2.1 1-L beaker dynamic	80, 94, 99	1, 3, 5, 10, 20, 30, 45, 60, 90	5, 25	5	1	3	18
3.2.2 300-mL beaker dynamic	94	3, 5, 8, 12, 20, 30	12, 14, 16, 18, 20	5	1	3	90
3.2.3 1-L beaker equilibrium	80, 85, 94, 99	60 (80°C), 45 (85°C), 30 (94°C), 20 (99°C)	2, 3, 4, 5, 6, 10, 13, 15, 20, 17, 25	2, 3, 4, 5, 6 (all at $R_{brew} = 15$)	1	3	99
3.2.4 Traditional cupping	99	14	12 to 21	10	5	3	90

*All grind size settings refer to Mahlkönig Guatemala Lab Grinder (cf. Supplementary Fig. S1), except for the traditional cupping which was performed on a Mahlkönig Guatemala 710 Grinder.

Table 2-1. Specific values of brewing parameters tested in four different brewing experiments. For the 1-L beaker equilibrium full immersion brews, selected combinations of brewing conditions present in Figure 3 were tested.

2-4.1 Coffee

For our systematic tests using 1-liter full immersion brews, we used a blend of four African-origin wash-processed Arabica coffees (Rwanda Kivu Kanzu, Rwanda Kivu Kibuye, Rwanda Musasa Mbilima Dukunde, and Ethiopia Yirgacheffe Kebele Kochore) procured from Royal Coffee in Oakland, CA. Each green coffee was roasted separately, and all were roasted at the UC Davis Coffee Center using a Loring demo roaster (Loring Smart Roast, Inc., Santa Rosa, CA, USA) within a 5-day period. The roast levels were 67.2, 70.0, 70.1, and 70.4 respectively, determined by the Agtron Gourmet Color Scale published by the SCA (Specialty Coffee Association, 2018). The coffee was allowed to rest for 2 days after roasting to allow for degassing, and then the four coffees were well-mixed together by hand, vacuum-sealed in 1-kg bags, and stored in a -20°C freezer. Each individual bag of coffee was defrosted overnight to room temperature before use.

For our dynamic tests with 300-mililiter brews, we used a single origin wash-processed Arabica coffee from Rwanda Kivu Kanzu provided by Royal Coffee in Oakland, CA. Coffee was roasted to an Agtron Gourmet reading of 70.1 at the UC Davis Coffee Center using a Loring demo roaster on a single day, followed by a 2-day resting period. Then, coffee was well-mixed, vacuum-sealed in 1-kg bags, and stored in a -20°C freezer; and individual coffee bag was defrosted in room temperature before use.

For our traditional cupping tests, five different commercially available blends of Arabica coffee were provided by Peet's Coffee (Alameda, CA, USA). Specifically, we tested Colombia Luminosa, Big Bang, Major Dickason's Blend, and French Roast, which respectively represent light roast, medium roast, dark, roast, and extra dark roast; note that a "light" roast at Peet's Coffee is typically darker than roasts characterized as "light" elsewhere. We also tested Decaf House Blend, a decaffeinated dark roast. Each coffee was roasted at Peet's Roastery in Alameda, CA using a Probat R-Series Solid Drum Roaster. The corresponding Agtron Commercial Color Scale readings were 54.6, 45.0, 35.1, 26.9, and 35.1, respectively. The coffees were ground and brewed on the same day of roasting, without packaging or a degassing period, to mimic standard quality control procedures.

2-4.2 Experimental Methods

2-4.2.1 Dynamics of extraction in 1-L Beaker Full Immersion Brews

Preliminary experiments assessed how much time was required to reach equilibrium. The dynamics of full immersion brewed coffee were studied at two different brew ratios and three different brew temperatures. Coffee was ground immediately prior to each experiment using a Mahlkönig Guatemala Lab Grinder (Mahlkönig USA, Durham, NC, USA) at grind size setting 5 with a median particle size ,x_{50}, of 1160.5 ± 28.8 µm. The particle size distribution (cf. Supplementary Fig. 2-S1) of each grind size setting from 2 to 6 were measured in triplicate using a Sympatec HELOS/RODOS T4.1 laser analyzer (Sympatec GmbH, Clausthal-Zellerfel, Germany) with the Sympatec Vibir vibratory feeder and R7 lens. Nestlé Pure Life Purified Water was used for all brews (Nestlé Waters North America, Inc., 2019). The pH of this water was measured to be 7.46 by Mettler Toledo SevenCompact Duo S213 pH/Conductivity Meter (Mettler-Toledo LLC, Columbus, OH, USA). Water was heated to a target temperature by an OXO Adjustable Temperature Pour-Over Kettle (OXO, New York City, NY, USA).

Water extraction temperatures were chosen at 80°C, the low end of brewing temperatures found acceptable by consumers for hot brewed coffee(Lee and O'Mahony, 2002); 94°C, within the range of brewing temperature suggested by the Coffee Brewing Handbook published by the Specialty Coffee Association(Lingle, 2011); and 99°C, as close as possible to boiling. The coffee was brewed using a 1-L glass beaker by adding an appropriate amount of water at 80°C, 94°C or 99°C to a constant amount of 30 g of coffee grounds to yield a desired brew ratio. Water was poured in a circular motion to ensure all the coffee grounds were fully wet. The timing of the brews started once water pouring was completed. The beaker sat on a room temperature wooden countertop with no lid; no additional insulation was provided to mimic typical brewing conditions. Accordingly, the temperature decreased after addition of the hot water to the room temperature grounds (cf. Supplementary Fig. 2-S2). At 1, 3, 5, 10, 20, 30, 45, 60 minutes for all brews, and 90 minutes for the $R_{brew} = 5$ brews, since it took longer for the brews at lower brew ratios to reach equilibrium. A single drop of coffee was pipetted out from the brew to measure the *TDS* at that time points stated above. Aside from this gentle sampling, no stirring was performed. All measurements were performed with three separate trial replicates.

2-4.2.2 Dynamics of extraction in 300-mL Beaker Full Immersion Brews followed by Filtration

Because the sampling could theoretically affect the extraction dynamics, we also performed tests where a 300-mL brew sat completely undisturbed until a specified brew time, at which point it was filtered through paper and then its *TDS* measured. The same coffee grinding procedure was used as with the 1-L beaker full immersion brews. Deionized water was heated using an OXO Adjustable Temperature Pour-Over Kettle (OXO, New York City, NY, USA) to 94°C.

The coffee was brewed using a 300-mL glass beaker by adding a constant amount of 200 g of water at 94°C to an appropriate amount of coffee grounds to yield a desired brew ratio. Water was poured in a circular motion to ensure all the coffee grounds were fully wet and the brew timing was started once the water pouring was completed. The beaker sat on a room temperature wooden countertop with no lid; no additional insulation was provided to mimic typical brewing conditions. At the end of 3, 5, 8, 12, 20, or 30 minutes into the brew, the whole brew including grounds and coffee were poured into a Hario V60 03 dripper and filter paper (Hario Co., Ltd, Chuo-Ku Tokyo, Japan), where the liquid coffee was separated from the spent grounds using a typical drip brew method with a drip-out time of 1 to 2 minutes. The mass of the liquid brew was weighed, then a small droplet was pipetted out for *TDS* measurement. All measurements were performed with three separate trial replicates.

2-4.2.3 Equilibrium in 1-L Beaker Full Immersion Brews

The previous two sets of experiments assessed the dynamics of extraction to identify how much time was necessary to achieve equilibrium. That information was then used to guide systematic tests of the impact of brew ratio, brew temperature, and grind size on the equilibrium *TDS* and extraction. Coffee was ground immediately prior to brewing using a Mahlkönig Guatemala Lab Grinder, typically at grind size setting 5 but also at settings ranging from 2 to 6, corresponding to extra fine to coarse. The median particle sizes are approximately 580, 780, 970, 1160, and 1310 μm at grind size setting 2, 3, 4, 5 and 6 respectively (cf. Supplementary Fig. 2-S1) . The same type of water (Nestlé Pure Life Purified Water) as for the dynamic experiments was heated using an OXO Adjustable Temperature Pour-Over Kettle to a specified temperature between 80°C to 99°C. Coffee was brewed using a 1-L beaker by adding an appropriate amount of water to a constant amount of 30 g of coffee grounds to yield a desired brew ratio. Water was poured in a circular motion to ensure all the coffee grounds were wet. The full immersion brew was left on wooden countertop at room temperature for a target brew time: 60 minutes for 80°C brew, 45 minutes for 85°C brew, 30 minutes for 94°C brew, and 20 minutes for 99°C brew, all time values at which the preliminary experiments indicated the *TDS* of the brew had reached a steady value. The temperature of the brew was measured using an OMEGA HH806AW Wireless Multilogger Thermometer (Omega Engineering, Inc., Norwalk, CT, USA).

After allowing the brew to equilibrate the coffee grounds were filtered out by slowly pouring the brew in a slightly tilted angle through a Hario V60 03 filter paper. The majority of spent coffee grounds remained in the beaker, though a small fraction moved with the brew onto the filter paper. After the brew finished draining through the filter paper, the filter paper and spent grounds on it were carefully returned to the 1-L beaker with the remainder of the spent grounds. The entire beaker, with spent grounds and filter paper, were then placed in an oven for drying. The mass of the filtered brew was weighed, and then a small droplet was pipetted out to measure the *TDS*. All measurements were performed with three separate trial replicates.

2-4.2.4 Traditional cupping in 12-oz Cup Full Immersion Brews

Finally, we performed systematic experiments to assess the strength and extraction of coffees prepared using the traditional cupping method. Coffee was grounded using a Mahlkönig Guatemala 710 Grinder at setting 10 with a median particle size at 548.3 ± 13.4 µm for all five of the coffee blends tested. Particle size distributions were measured by the same laser analyzer in triplicate for each coffee blend. Coffee was brewed on the same day of roasting. All coffees were cupped with filtered water containing 180 ppm of dissolved ions, within in the standard range specified by SCA standards. Coffees were brewed individually in a 12-oz glass cup by adding approximately 180 g of 99°C water to a target amount of coffee grounds, 9 to 14 g, to yield a desired brew ratio. All masses were weighed after adding coffee grounds and adding the water to provide the precise brew ratio. Water was heated using a Bonavita 1.7-L Variable Temperature Electric Kettle (Bonavita World, Woodinville, WA), and was poured in circular motion to ensure all coffee grounds were wet. As per the traditional protocol, four minutes after the brew began a cupping spoon was used to push down and submerge the grinds that had risen to the top layer of the liquid. After that, the brew was left at room temperature for another 10 minutes; then, a Hario V60 02 filter paper was used to filter out the spent coffee grounds from liquid coffee. After the liquid coffee cooled down to room temperature, a small drop of brew was pipetted out to measure the *TDS*. All measurements were performed with three separate trial replicates.

2-4.2.5 Quantitative measurements

2-4.2.5.1 Extraction Yield Calculation

Brew ratio R_{brew} was calculated with experimental mass measurements of fresh coffee grounds and water using equation (2-1). E was calculated from experimental *TDS* measurements and R_{brew} using equation (2-16).

2-4.2.5.2 Oven Drying Mass Measurements

An overview of the experimental procedure involving oven drying method is illustrated in Fig. 2-1. The 1-L beaker containing spent coffee grounds along with the filtered paper was oven-dried at 100°C for 24 hours. After that, the mass of the whole beaker was measured using a Mettler Toledo PC 2000 Digital Lab Balance (Mettler-Toledo LLC, Columbus, OH, USA). The mass of the dried coffee grounds M_{dried} was obtained by subtracting the masses of the beaker and filter paper, each measured prior to coffee brewing. Then, E_{oven} was calculated using equation (2-17). The retention ratio R_{ret} was calculated as per equation (2-23) from the measured *TDS* and the mass measurements of water, fresh coffee grounds before brewing, and liquid coffee beverage after filtration.

2-4.2.5.3 Digital Refractometer Calibration

The *TDS* of liquid coffee at room temperature was measured using a digital refractometer (VST, Inc). The refractometer was zeroed with distilled water prior to experimental measurements. Calibration of the digital refractometer was performed using soluble Nescafé Clasico Dark Roast Instant Coffee, by dissolving a specified mass ranging from 0.5 to 4 g of instant coffee in 100 °C deionized water. The mass of instant coffee was measured using a Fisher Scientific XA Analytical (Thermo Fisher Scientific, Waltham, MA, USA). The actual *TDS* was calculated by mass as

$$TDS_{calc} = \frac{mass\ of\ instant\ coffee}{mass\ of\ instant\ coffee + mass\ of\ water} \times 100\%, \qquad (2\text{-}24)$$

and the measured *TDS* of the solution was measured at room temperature using a VST digital refractometer. The resulting calibration curve (Supplementary Fig. 2-S3) indicates that the refractometer yields excellent measurements of the *TDS*. All *TDS* values reported here are those as measured by the refractometer.

2-4.3 Data Analysis

Nonlinear regression of *TDS* to R_{brew} via equation (2-10) was performed using the MATLAB built-in function *lsqcurvefit*, using K as the regression parameter. The corresponding best-fit parameters were evaluated using the built-in function *nlparci* to return a 95% confidence interval. Linear regressions of E_{oven} via equation (2-21), *TDS* calibration, and *TDS* and *E* over grind particle size were performed using built-in function *polyfit*. The correlation coefficient (*R*) and p-value of the corresponding linear regressions were calculated using the built-in function *corrcoef*. All plots were generated using MATLAB R2020b (The MathWorks, Inc., Natick, MA).

2-5. Results

2-5.1 Dynamics of extraction

Our dynamic experiments with 1-L brews show that the *TDS* of full immersion brewed coffee increases with brew time then plateaus after approximately 20 minutes, for all brew ratios at all brew temperatures tested. For the 1-L full immersion dynamic extractions, coffee brewed with a lower brew ratio yielded higher *TDS* values, as expected, due to the higher concentrations of soluble species present in the brew, but also took slightly longer to reach equilibrium since the concentration gradient as driving force is smaller between solid and liquid phase compared to the brews with higher brew ratio. For $R_{brew} = 25,$ steady *TDS* values of approximately 0.7% *TDS* were obtained in 20 minutes for all brew temperatures tested. In contrast, for $R_{brew} = 5$ the brews reached an averaged equilibrium *TDS* value of approximately 4% at around 45 minutes into the brew. Similar results were observed with our 300-mL full immersion brews with a single *TDS* sampling after filtration (Fig. 2-2b). Brews with R_{brew} ranging from 12 to 20 reached steady *TDS* values ranging from approximately 1.65% to 0.95%, respectively, within about 20 minutes.

Coffee brewed with higher temperature water reached a steady *TDS* value more quickly than lower temperature brews did (Fig. 2-2a). The 99°C brew with $R_{brew} = 5$ exceeded 4% *TDS* within 20 minutes, while the 94°C and 80°C brews took more than 30 minutes to reach comparable values. Even though the brew temperature did affect the dynamics of full immersion brewed coffee, it did not appreciably affect the final equilibrium *TDS*. Based our 1-L full immersion brews results, coffee brewed at $R_{brew} = 5$ had a mean and standard deviation of $4.07\% \pm 0.15\%$ *TDS* regardless of brew temperature, and *TDS* was $0.75\% \pm 0.04\%$ for coffee brewed at $R_{brew} = 25$ over the range of 80 to 99°C.

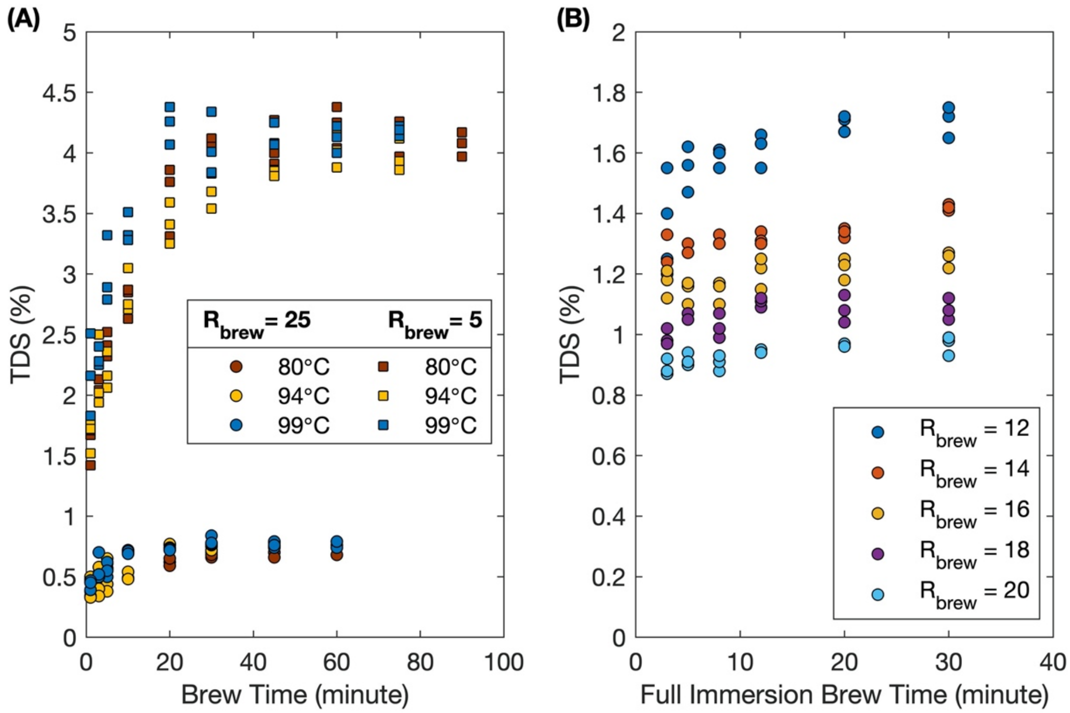


Figure 2-2. A) Dynamics of extraction for 1-L full immersion brews at two different brew ratios ($R_{brew} = 5$ and $R_{brew} = 25$) and three different brew temperatures (99°C, 94°C, and 80°C). Scatter plot *TDS* vs. brew time of full immersion brews with at brew temperatures. Each experiment was performed in triplicate. **B)** Dynamic *TDS* vs. full immersion brew time of 300-mL beaker full immersion brews followed by a filtered drip brew at five different brew ratios.

2-5.2 Equilibrium TDS and E in 1-L Brews

After our dynamic tests allowed us to identify conservative over-estimates of the time required to reach equilibrium *TDS* values, we systematically tested the impact of brew ratio at different brew temperatures and grind sizes to test model prediction equation (2-10). The results are plotted in Fig. 2-3, which illustrates that the equilibrium *TDS* is indeed inversely proportional to R_{brew}, regardless of the brew temperature or grind size over the ranges tested. This finding is consistent with the equilibrium *TDS* values in the dynamic extraction of full immersion brews (cf. Fig. 2-2a). Our model (cf. Eq. 10) yields an excellent fit versus R_{brew} from nonlinear regression, where the best-fit value of equilibrium constant K is 0.717 ± 0.007 with 95% confidence interval over wide range of brewing conditions. This calculation for K assumes that $E_{max} = 0.3$ is known with perfect confidence; if we instead treat the quantity KE_{max} as a lumped unknown parameter, then regression yields $KE_{max} = 0.215 \pm 0.002$. The inset in Figure 2-3 shows the same *TDS* data plotted versus $1/R_{brew}$ to test the approximate inverse dependence (Eq. 11). The linear fit is excellent, with correlation coefficient R=0.999 and corresponding p-value 3.66×10^{-105}, indicating that Eq. 11 provides an accurate approximation.

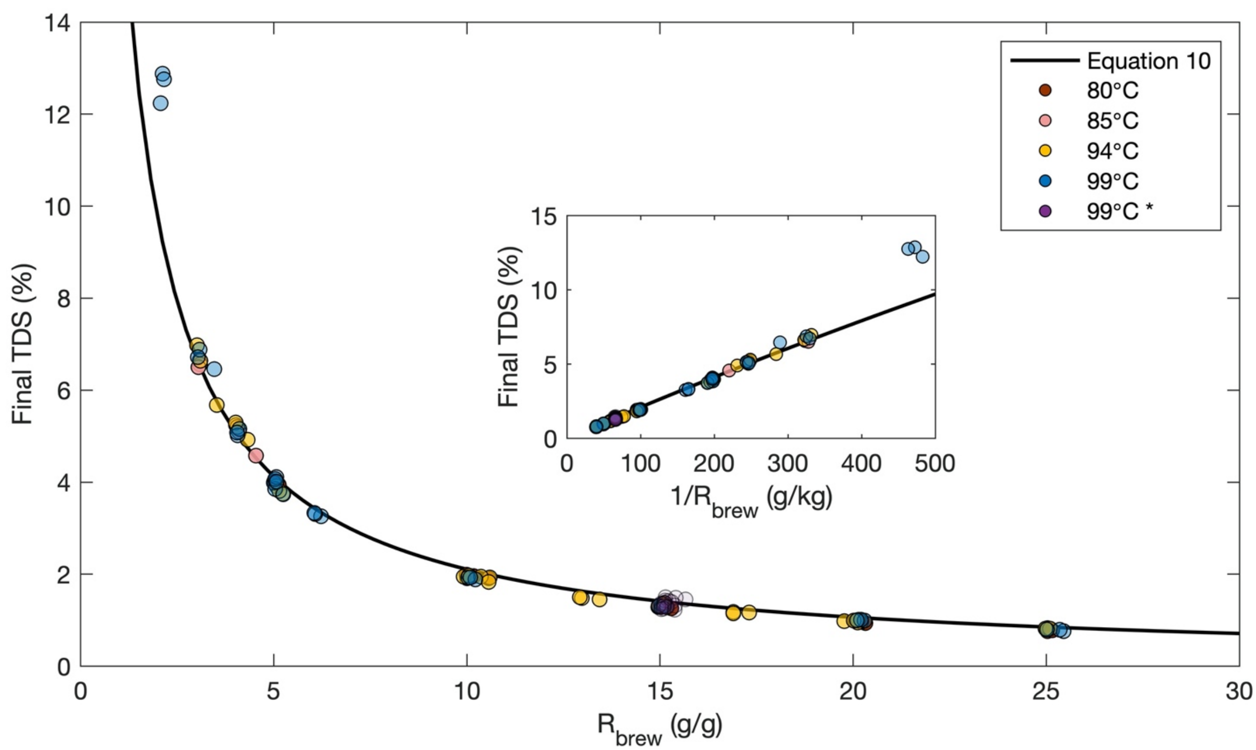


Figure 2-3. Equilibrium *TDS* vs. brew ratio for 1-L full immersion brews at various brew temperatures and grind sizes. The asterisk in legend denotes brews with wide range in grind particle sizes (cf. Supplementary Fig. S4). Solid black line is the adsorption-desorption model prediction (Equation 2-10), where $E_{max} = 30\%$, and the equilibrium constant $K = 0.717 \pm 0.007$ was determined by nonlinear regression with $R_{brew} > 3$ data points. All experiments were performed in triplicate; a total of 99 distinct *TDS* values are plotted here. Inset shows the same data and model fit, plotted versus the inverse brew ratio.

The most surprising finding is that K did not change appreciably with respect to brew temperature from 80 to 99°C. The coffee grind particle size did have a very minor effect on *TDS*. For the brews at $R_{brew} = 15$ at 99°C, both the equilibrium *TDS* and *E* are negatively correlated with the median of grind particle size with a correlation coefficient of -0.978 and -0.992 (solid lines in Supplementary Fig. 2-S4), that is, coffee brewed with finer coffee grounds resulted in slightly higher *TDS* and E. The *TDS* was $1.36\% \pm 0.09\%$ over a huge range of grind particle sizes, from a median particle size of 579 μm to 1311 μm (cf. Supplementary Fig. 2-S1), but these small *TDS* differences are difficult to discern compared to the major effect of R_{brew} over the entire range of brew ratios tested.

Equation (2-10) fit the data extremely well everywhere except at the extreme value of $R_{brew} = 2$, which had a higher *TDS* than predicted. Importantly, this brew ratio is less than the average retention ratio of 2.48 ± 0.19 calculated from equation (2-23), i.e., it is unclear that adding only 2 grams of water for every gram of coffee grounds is adequate to fully wet the coffee grounds. Qualitatively, at $R_{brew} = 2$ the grounds looked like more like a moist sludge than a “fully immersed” brew. Accordingly, we excluded these three data points from the nonlinear regression.

The corresponding extraction yields for the 1-L brews are shown in Fig. 2-4. Two different types of extraction measurements are shown here, based on different experimental measurements. First, the “equilibrium extraction” (round data points) are based on the *TDS* measurements at equilibrium and the known brew ratio, and calculated via equation (2-16). We emphasize that only the *TDS* values and R_{brew} inform these calculated equilibrium extraction values; no drying data or best fit K values are involved. The averaged equilibrium E calculated in this manner is $20.70\% \pm 1.08\%$ for $R_{brew} \geq 3$ (again excluding the 'moist sludge' results at $R_{brew} = 2$) . This result is in excellent agreement with the theoretical prediction of equation (2-14), $E = KE_{max}$, which based on the nonlinear regression described in Fig. 2-3 is $E = 21.5 \pm 0.2\%$ (solid black line, Fig. 2-4).

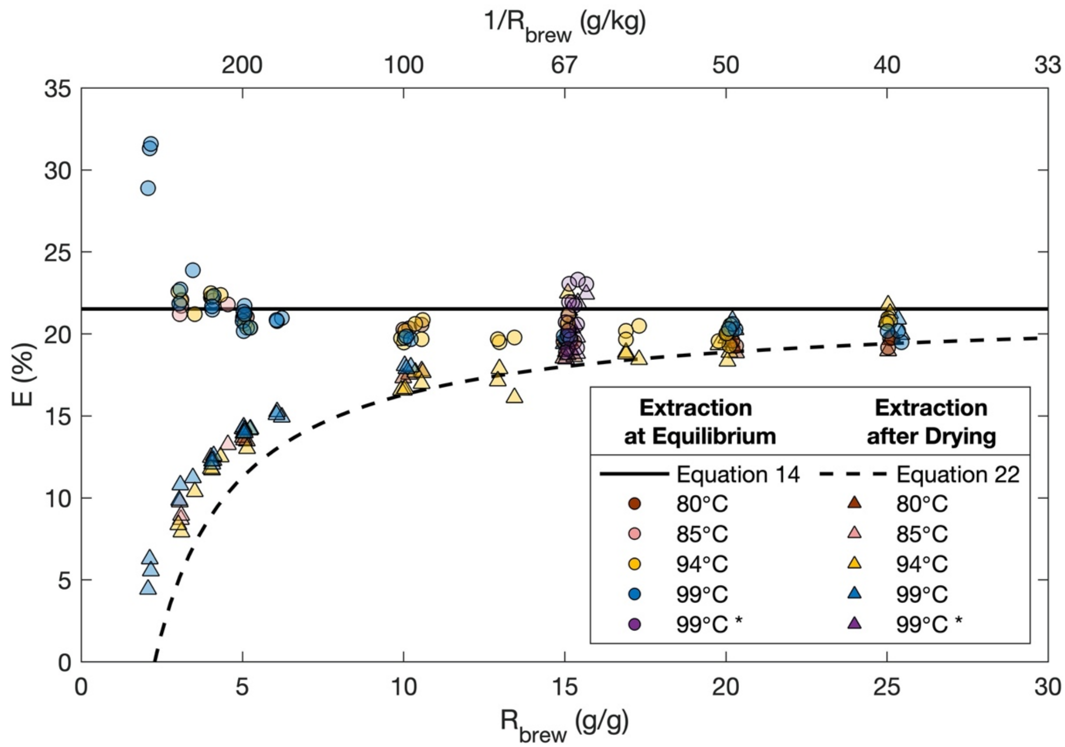


Figure 2-4. Equilibrium E vs. brew ratio for 1-L full immersion brews at various brew temperatures and grind sizes. The asterisk in legend denotes brews with wide range in grind particle sizes (cf. Supplementary Fig. S4). A secondary x-axis indicates the inverse brew ratio. Solid black line is the adsorption-desorption model prediction for extraction yield (Equation 2-14), and the dashed black line is the adsorption-desorption model prediction for oven drying extraction yield (Equation 2-22), where $E_{max} = 30\%$, and the equilibrium constant $K = 0.717$. All experiments were performed in triplicate; a total of 99 distinct data points for both E and E_{oven} are plotted here.

The second kind of extraction yield measurements were those obtained by oven drying (triangles in Fig. 2-4). These E_{oven} data points involved only mass measurements of the grounds before brewing and after oven-drying, as per equation (2-17). As expected, E_{oven} increased with the brew ratio, then plateaued around 20%, where it approached the values of the equilibrium E. This finding is also consistent with the theoretical prediction (dashed black line, cf. Eq. 22), because a much larger fraction of dissolved coffee species was left in the retained coffee in the moist spent grounds; in other words, R_{ret}/R_{brew} is larger at low R_{brew} than in high R_{brew} resulting in a smaller value of E_{oven}. Notably, there appears to be a small but systematic gap between the experimental E_{oven} data points and the model prediction curve for E_{oven}. This effect is presumably due to the exclusion here of the volatilization ratio, which the averaged and standard deviation calculated using Equation (2-19) is $R_{vol} = 0.0234 \pm 0.006$. As a comparison, a linear regression of E_{oven} via the desorption model prediction (Equation 2-21) gives a regressed value of $R_{vol} = 0.0228$ as the intercept of the best-fit line (Supplementary Fig. 2-S5). In other words, these data suggest that a little more than 2% of coffee solid mass is volatilized during oven 24 hours of baking at 100 °C.

Furthermore, we found that the finer the grinds, the higher the observed values of both E and E_{oven}, at least for a constant brew ratio (Supplementary Fig. 2-S4b). The observed spread, however, was within 4% (i.e., E ranged from about 19 to 23%), over a huge span of coffee particle sizes. Therefore, variation in brew temperature or grind sizes did not considerably alter the extraction yield either for full immersion brewed coffee.

2-5.3 Equilibrium TDS and E in Traditional Cupping

Because coffee cupping is one of the most important techniques the coffee industry uses to evaluate coffee quality, full immersion brews following recommended cupping protocol were also investigated systematically versus brew ratio. We again find the final *TDS* is inversely proportional to brew ratio for all five different roast levels tested (Fig 2-5a). Surprisingly, the four regular coffees tested, ranging from light roast to extra dark roast, had effectively indistinguishable equilibrium *TDS* values. In contrast, the *TDS* of the decaffeinated coffee was systematically lower than the regular caffeinated coffee, presumably because it lost some soluble mass when it went through a caffeine extraction process prior to roasting (Ramalakshmi and Raghavan, 1999). The regressed equilibrium constants K with 95% confidence interval from our desorption model (cf. Eq. 10) are 0.792 ± 0.004 for caffeinated coffee and 0.726 ± 0.006 for decaffeinated coffee, again assuming $E_{max} = 0.3$ with perfect confidence; the corresponding lumped parameters are $KE_{max} = 0.240 \pm 0.002$ for caffeinated and $KE_{max} = 0.218 \pm 0.002$ for decaffeinated. The inset in Fig. 2-5a shows the same data plotted versus $1/R_{brew}$ to test Eq. (10), and as in Fig. 2-3 the linear fit is excellent (R=0.992, p=6.037×10^{-80} and R=0.997, p = 6.899×10^{-24} for caffeinated and decaffeinated coffee, respectively).

Our corresponding measurements of the equilibrium extraction yield (using equation 2-16) again corroborate the model prediction that the extraction yield is insensitive to brew ratio (Fig. 2-5b). The experimental averaged equilibrium E values with standard deviation are $23.9\% \pm 0.6\%$ for caffeinated coffee regardless of roast level and $22.2\% \pm 0.4\%$ for decaffeinated coffee, which accord with our model prediction of 23.79% and 21.79% for caffeinated and decaffeinated coffee, respectively (solid lines, Fig. 2-5b).

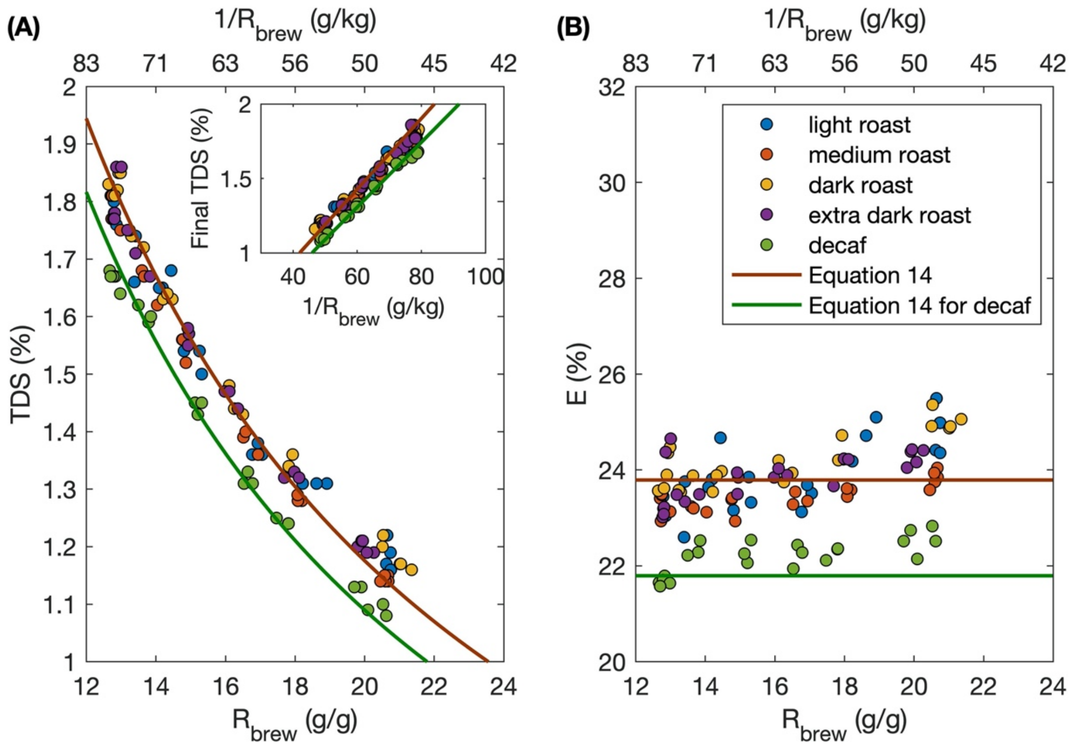


Figure 2-5. A) Regression of final *TDS* vs. R_{brew} of traditional cupping full immersion brews using different coffee at various roast levels to the adsorption-desorption model, where $E_{max} = 30\%$ and the equilibrium constant K serves as the fitting parameter. The best-fit K values with 95% confidence interval are 0.792 ± 0.004 for caffeinated coffee 0.726 ± 0.006 for decaffeinated coffee. **B)** Scatter plot of E vs. R_{brew} and model prediction (Equation 2-14) for traditional cupping full immersion using different coffee at various roast levels.

2-6. Discussion and Conclusions

The overarching conclusion from this work is that full immersion coffee brewing is well characterized by an equilibrium desorption model that assumes not all of the soluble material in the coffee grounds will go into solution. The experimental measurements of *TDS* and E over a wide range of conditions strongly accord with the model predictions, indicating that use of a single averaged equilibrium constant suffices to capture the overall behavior of the complicated mixture of individual chemical components.

2-6.1 Insensitivity to Temperature

A surprising aspect of our results is the pronounced insensitivity to the brew temperature. Although the dynamics of extraction were strongly affected by the brew temperature, with hotter temperatures yielding an equilibrium *TDS* more quickly than lower temperatures (Fig. 2-2a), the final value of the *TDS* and corresponding E were insensitive to the brew temperature over the wide range 80 °C to 99 °C. We emphasize, however, that this result does not mean that the brews prepared at these different temperatures will necessarily taste the same. The sensory impressions perceived by individuals upon tasting the brew depend on the concentration of individual chemical species within it, not the overall mass fraction of dissolved solids; it is possible that two brews could have the same *TDS* and E but nonetheless have different underlying chemical compositions and hence different sensory profiles. Furthermore, measurements of the *TDS* do not reflect the presence of emulsified oil droplets or non-dissolved colloids, both of which affect the sensory profile and conceivably could vary more dramatically with brew temperature.

Despite these caveats, however, there is reason to suspect that the brew temperature might not appreciably alter the final sensory profile full immersion brews. Work by Batali et al.

demonstrated that drip brew coffees prepared to identical *TDS* and E values but using different brew temperatures had sensory profiles that were indistinguishable to trained panelists(Batali et al., 2020a). Although those drip brew experiments were performed over a narrower temperature range (87 °C to 93 °C), they raise the possibility that a similar lack of sensory profile dependence on brew temperature might occur with full immersion brews over a wider range of temperatures. Detailed sensory descriptive experiments must be performed with full immersion brews to test this hypothesis. Furthermore, the tests reported here did not examine "cold brews," which are traditionally performed either at room temperature (near 24°C) or refrigerator temperature (near 4°C). Additional experiments are necessary to examine the behavior of full immersion cold brew.

2-6.2 Strength and Extraction Control via Brew Ratio

Although the brew temperature over traditional hot brew temperature ranges might not affect the final brew appreciably, our results clearly demonstrate that the brew ratio has a huge influence: our model and experimental results both indicate that the *TDS* varies inversely with R_{brew}. Because the sensory profile is strongly correlated with the *TDS*, this result indicates that the simplest way to modify the sensory profile for full immersion brewing is to modify the brew ratio. Changes in the brew temperature, grind size, and agitation will alter the dynamics of the extraction, but not the composition of the final brew itself; in contrast, the brew ratio directly controls the final composition.

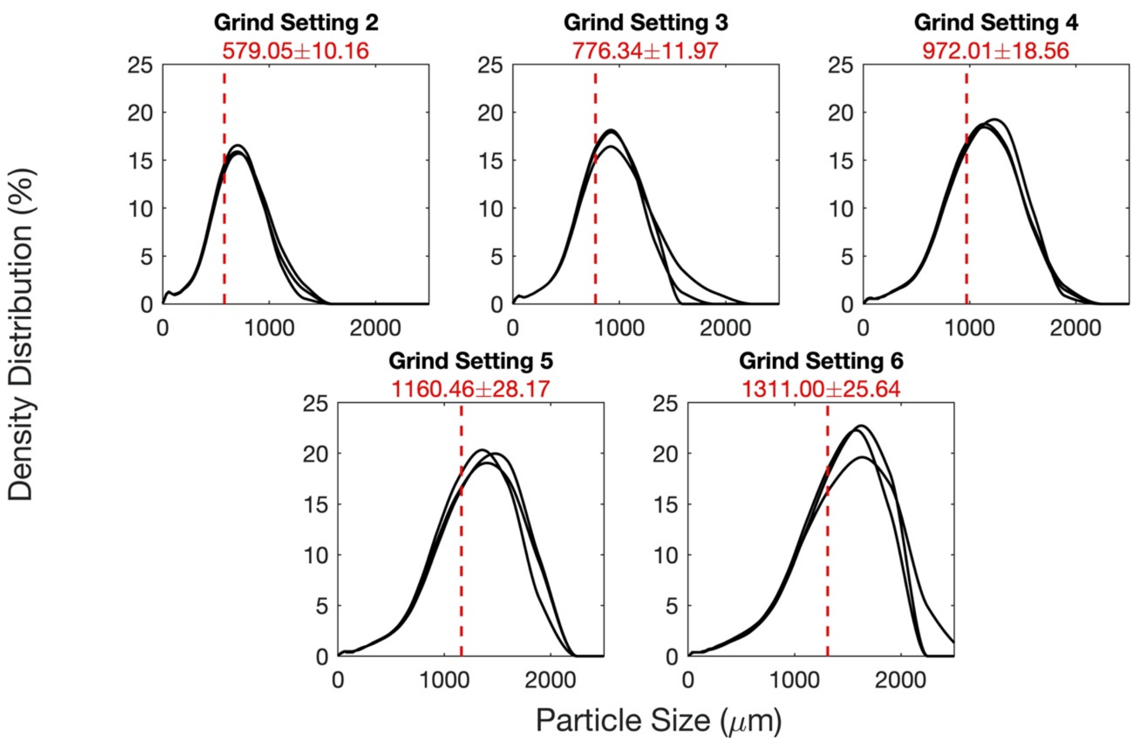
In contrast to the ease with which *TDS* is varied, our results indicate that full immersion brewing offers little control over the extraction yield. To good approximation over typical brew ratios, the *E* is predicted to be independent of the brew ratio (cf. Eq. 14). Specifically, based on our measurements, it appears that full immersion brews at equilibrium invariably yield an E near 21%, and modifications in the brew temperature, grind size, or brew ratio do not alter the final E appreciably. We emphasize that this "equilibrium E" is what matters for the beverage because it directly corresponds to the beverage that is to be consumed, whereas the effective E measured via oven drying is potentially misleading because it includes dissolved but retained mass in the filtered spent coffee grounds and thus provides a significant underestimate of the actual E in the beverage.

Another notable observation is that the traditional cupping brews had a slightly higher K and E than the 1-L beaker equilibrium brews. The reason for this difference is unclear. One possible confounding factor is that the coffees for the traditional cupping tests were brewed the same day that they were roasted, without a lengthy degassing period as allowed for the 1-L tests reported here. The release of CO_2 and other volatile compounds happens with a varied degassing speed depending on the roast level and roast speed, and can cause mass losses on the order of 10 mg/g of roasted coffee, equivalent to a 1% mass loss (Smrke et al., 2018). If, however, these volatile species were still present in the roasted beans when weighed, but then they readily escape into the gas phase upon brewing, then the extraction yield should be lower, rather than higher as observed. Another possible factor is that slow chemical reactions continue to occur after roasting (Clarke and Macrae, 1987); if these reactions alter the solubility or equilibrium desorption coefficients, then the average equilibrium *TDS* and extraction yield will be affected accordingly. More specific tests will be necessary to test this hypothesis.

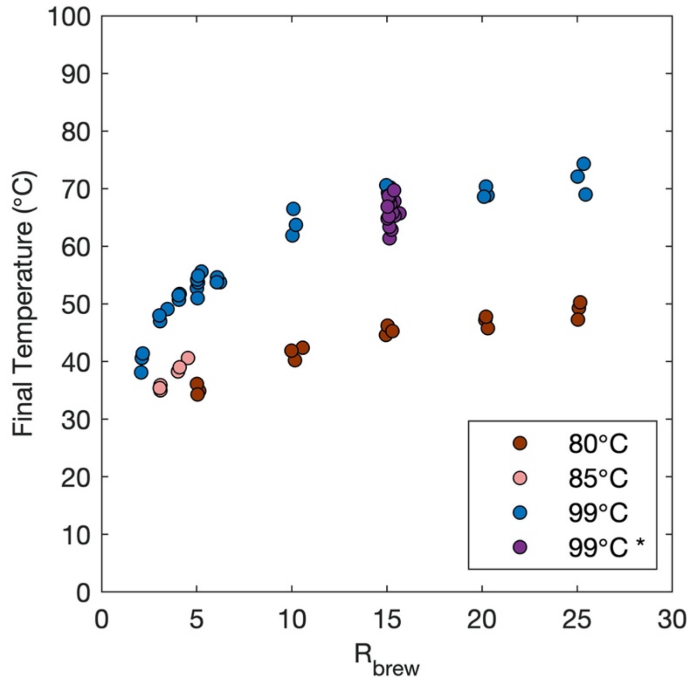
2-6.3 Implication for Practitioners

In terms of practical implications, the inability to alter the equilibrium E in full immersion brews effectively removes a “knob” available to fine tune the desired sensory profile. Prior work with drip brews has shown that brews prepared at the same *TDS* but different E have significantly different sensory profiles.(Frost et al., 2020) In terms of the classic Coffee Brewing Control Chart, full immersion brews at equilibrium only allow a brewer to move vertically with respect to *TDS* (by changing the brew ratio), but not horizontally with respect to E. This observation suggests the hypothesis that full immersion techniques cannot easily produce brews with maximum amounts of sourness and citrus (as observed with low E, high *TDS*) or maximal amounts of sweetness (as observed at low *TDS*, low E) or maximal amounts of tea/floral (as observed at low *TDS*, high E). Lower E values can be obtained in full immersion only by cutting the brew short (i.e., not allowing it to reach a final steady *TDS* value); higher E values cannot be obtained with a single full immersion brew. In contrast, flow brewing methods like drip brew provide more flexibility, since the flow rate, brew ratio, and total brew time can be varied to achieve desired combinations of *TDS* and E. This increased flexibility, however, is potentially offset by the increased expense and complexity of drip brew equipment; cupping for example is widely preferred by coffee industry professionals because of its simplicity. Coffee brewers should take this tradeoff between flexibility and simplicity into account when choosing between flow based and full immersion brewing methods.

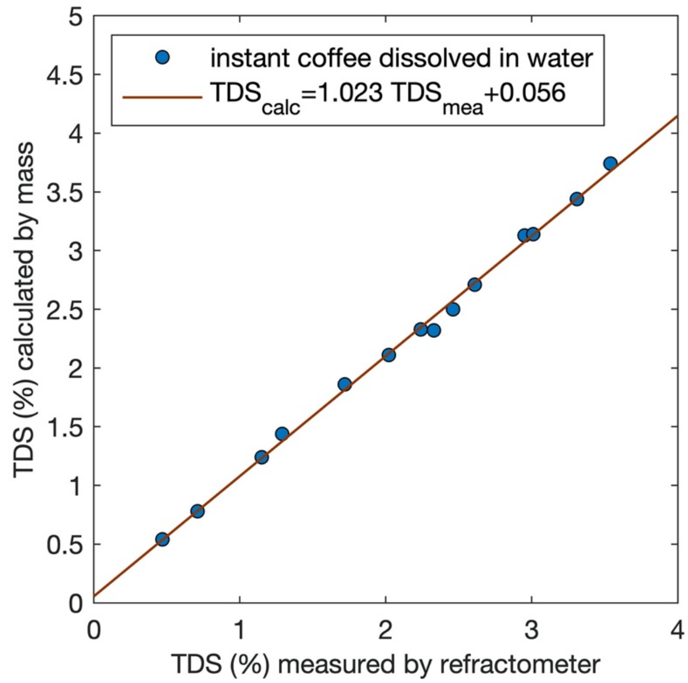
Supplementary Materials



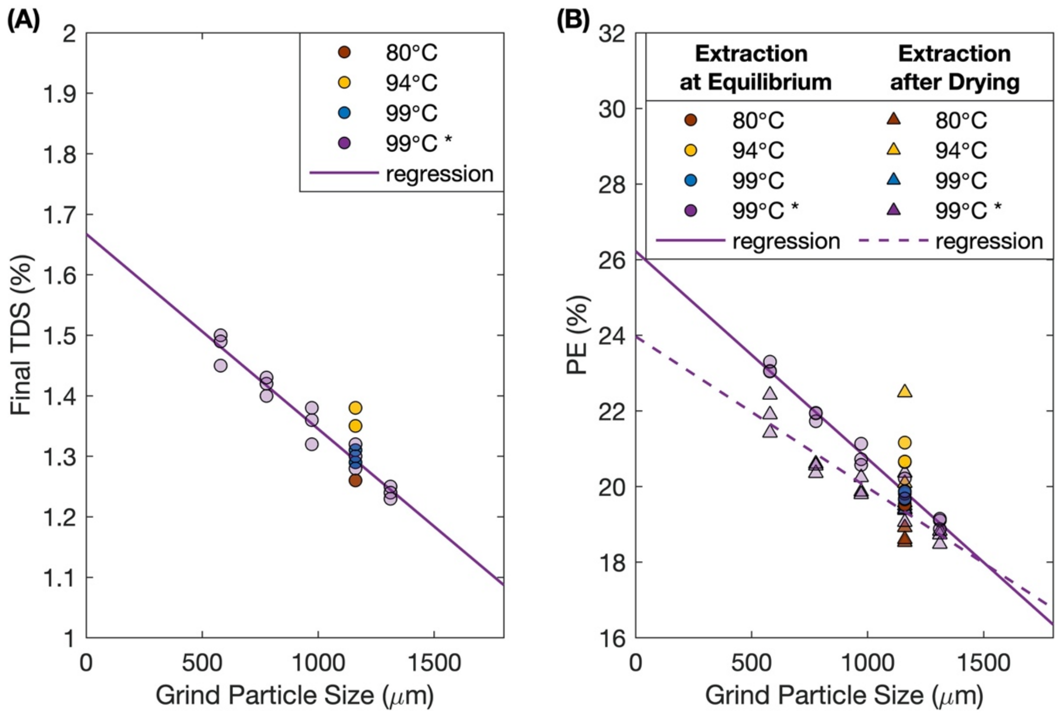
Supplementary Figure 2-S1. Particle size distribution at five different grind size settings for the Mahlkönig Guatemala Lab Grinder, each measured in triplicate. Distributions are expressed in terms of the normalized differential density distributions of the given particle size. The median particle size, x_{50}, with standard deviation at each grind size setting is indicated by red dashed line.



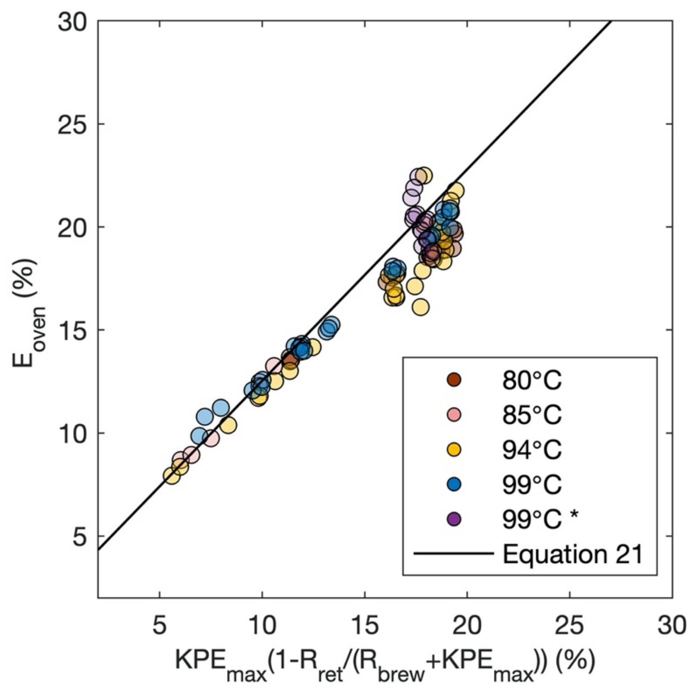
Supplementary Figure 2-S2. Final temperature vs. R_{brew} of 1-L full immersion brews at various brew temperature and grind sizes.



Supplementary Figure 2-S3. Calibration of *TDS* measurement from VST Digital Refractometer by linear regression from the calculated *TDS* value by mass TDS_{calc} using Equation 2-24 and the measured *TDS* value TDS_{mea} of dissolved pure instant coffee in boiling water. The correlation coefficient between TDS_{mea} and TDS_{calc} is 0.999, and the p-value is 8.818×10^{-17}.



Supplementary Figure 2-S4. (A) Equilibrium *TDS* vs. median particle grind size, x_{50}, (cf. Supplementary Fig. S1) for 1-L full immersion brews at $R_{brew} = 15$. The solid line denotes the linear regression $TDS = -0.0003x_{50} + 1.67$, for the brews at 99°C, with R= -0.978, p= 2.40×10^{-12}. (**B)** Equilibrium *E* vs. median particle grind size, for 1-L full immersion brews at $R_{brew} = 15$. The solid and dashed lines indicated linear regressions for E and E_{oven}, respectively, at 99°C, with corresponding equations $E = -0.0055x_{50} + 26.2$ and $E_{oven} = -0.0039x_{50} + 23.9$, The corresponding regression statistics are, respectively, R=-0.992, p= $7.21 \times 10^{-16}$and R=-0.933, p= 1.65×10^{-8}.



Supplementary Figure 2-S5. Equilibrium E_{oven} vs. $KE_{max}\left(1-\frac{R_{ret}}{R_{brew}+KE_{max}}\right)$ of 1-L full immersion brews at various brew temperatures and grind sizes. The asterisk in legend denotes brews with wide range in grind particle sizes, cf. Supplementary Fig. S4. Solid black line is the adsorption-desorption model prediction for Equilibrium E_{oven} (Equation 2-21) with $E_{max} = 30\%$, and the volatization ratio $R_{vol} = 0.0228$ was determined by the intercept of this best-fit line with slope $= 1.03$ through linear regression (R=0.997, p=1.10×10^{-38}). As a comparison, the averaged volatilization ratio with standard deviation calculated from Equation 2-19 using measurable quantities is $R_{vol} = 0.0234 \pm 0.006$.

Symbol	Units	Definition
C_A	-	mass concentration of adsorbed soluble coffee species
C_D	-	mass concentration of dissolved soluble coffee species (*TDS*)
C_{tot}	-	total concentration of extractable coffee species
E	-	extraction yield at equilibrium
E_{max}	-	maximum possible extraction yield of coffee grounds
E_{oven}	-	measurable extraction yield using the oven-drying method
K	-	species-averaged equilibrium constant
k_A	$1/\text{second}$	first order rate constant for adsorption of soluble species
k_D	$1/\text{second}$	first order rate constant for desorption of soluble species
M_A	grams	mass of adsorbed coffee species
M_{brew}	grams	mass of liquid beverage that could be consumed
M_D	gram	mass of dissolved coffee species
M_{dried}	grams	mass of dried spent grounds after oven drying
M_g	grams	Initial mass of coffee grounds added to the brewer
M_L	grams	mass of liquid present in the brew after dissolution of soluble species
M_{ret}	grams	mass of retained liquid coffee within the moist spent coffee grounds
M_{spent}	grams	mass of spent moist coffee grounds
M_{vol}	grams	mass of volatile coffee solids lost to the gas phase during oven drying
M_w	grams	Initial mass of water added to the brewer
R_{brew}	-	water to coffee mass brew ratio
R_{ret}	-	retention mass ratio (retained liquid per mass coffee grounds)
R_{vol}	-	volatilization mass ratio (evaporated solids per mass coffee grounds)
TDS	-	total dissolved solids (mass dissolved solids per mass of liquid)
x_{50}	μm	median of particle grind size distribution

Supplementary Table 2-S1. Table of nomenclature. A hyphen under “Units” denotes a dimensionless quantity.

Chapter 3. A diffusion-limited model for the extraction dynamics of full immersion brewed coffee under temperature, roast level, and origin effects

---

Author contributions:

Jiexin Liang co-designed the study, conducted experiments, performed data analysis and figure preparation, and wrote the original draft the manuscript. Lik Xian Lim and Angela L. Weber conducted experiments. Mackenzie E. Batali co-designed the study and conducted the experiments. Juliet Han co-designed the study and roasted the coffee. William D. Ristenpart secured funding, co-designed the study, advised data analysis, revised and edited the manuscript.

3-1. Abstract

We report that full immersion coffee brews conducted over a wide range of coffee preparation factors all follow the same "universal brewing curve" for the total dissolved solids (*TDS*) versus brew time. We propose an updated and extended diffusion-limited mass transfer model, experimentally validated with more than 3,000 *TDS* measurements, to predict the *TDS* and corresponding extraction yield of full immersion brewed coffee in terms of three parameters: an initial "rinse" concentration (C_0), an equilibrium concentration (C_{eq}), and an effective mass transfer coefficient (k). Systematic experimental measurements over a range of brew temperatures (4°C, 22°C, 94°C), roast levels (light, medium, dark), and coffee types (washed Ethiopian coffee, honey-processed coffee from El Salvador, and wet-hulled Sumatra coffee) establish that the *TDS* follows the universal brewing curve with appropriate values of C_0, C_{eq}, and k. As expected, we find that increasing brew temperature strongly increases the extraction rate, but we also find that the "rinse ratio" C_0/C_{eq} is positively correlated with brew temperature. Surprisingly, we observe that light roast beans extract much more quickly than dark roast, and we observe that the different coffee types yielded no statistically significant differences in extraction dynamics. We anticipate that the results presented here will help coffee practitioners select optimal brewing conditions to obtain desired *TDS* values and corresponding sensory qualities.

3-2. Introduction

Full immersion methods of brewing are widely used for coffee. It is most famously used for French press brewing and for cold brew, but practitioners within the coffee industry also heavily rely on a traditional full immersion method called "cupping" to assess coffee quality (Specialty Coffee Association, 2022, 2021). Full immersion brewing might seem simple since it only involves directly adding water to coffee grounds in a container, but it features a multitude of complicated physical effects and chemical effects that result in complex sensory profiles for different coffees (Spencer et al., 2016; Sunarharum et al., 2014). Much recent research has established that the sensory quality and consumer hedonic preferences of brewed coffee are highly correlated with the strength, also known as the total dissolved solids (*TDS*), and extraction yield (*E*) of the brew (Batali et al., 2022, 2020b; Cotter et al., 2021; Frost et al., 2020; Guinard et al., 2023; Lockhart et al., 1957). Thus, establishing the impact of coffee preparation factors on the extraction dynamics, measured in terms of *TDS* and *E*, is crucial to obtain desired sensory profiles.

Despite the widespread use of full immersion brewing, most prior research on extraction dynamics has focused on filtered drip brew and espresso (Cameron et al., 2020; Cordoba et al., 2020; Fasano and Talamucci, 2000; Gloess et al., 2013; Melrose et al., 2018), and there is comparatively less data on the extraction dynamics of full immersion coffee brewing (Liang et al., 2021; Moroney et al., 2016, 2015; Zanoni et al., 1992). Nevertheless, some key factors in the extraction dynamics of full immersion coffee brewing are well-established, such as how higher brewing temperature and finer grind size increase the rate of solubles extraction (Cordoba et al., 2020, 2019; Fuller and Rao, 2017; Voilley and Simatos, 1979). Other factors are less clear. Our previous study of full immersion coffee brewing investigated the effect of five different roast levels, with the results indicating that the roast level has little impact on the equilibrium *TDS* (Liang et al., 2021). Similarly, Cordoba et al. also found that the impact of roast level on final *TDS* is not significant when the same brewing method and brew temperature are used (Córdoba et al., 2021). Conversely, Rao et al. found that roast level did have a significant effect on final *TDS*, although it is unclear whether their coffee brews reached equilibrium at the time that *TDS* was measured (Rao et al., 2020). Furthermore, the coffee origin, i.e., where the coffee is grown under different conditions and post-harvest processed with different methods, has unclear impact on extraction dynamics. Cordoba et al. reported that different origins within the same producing country yielded insignificant differences in extraction dynamics under consistent brewing protocols (Cordoba et al., 2019). Coffees produced within the same country, however, tend to be processed similarly in contrast to the vast different post-harvest processing methods (e.g., washed, natural, honey, wet-hulled) used in different coffee producing origins across continents. It remains unclear how origin, processing method, and roast level affect the extraction kinetics of full immersion brewing techniques.

To address this point, a model to capture, compare, and predict the extraction dynamics of all soluble substances in full immersion brewed coffee is desirable. Towards that end, a few groups have developed theoretical models aimed at predicting the brew strength and extraction yield of full immersion brews. Early work by Voilley and Simatos suggested the extraction of coffee can be modeled by the classic diffusion equation to obtain an effective diffusion coefficient of all soluble solids via experimental measurements (Voilley and Simatos, 1979). They reported that the extraction yield reaches 90% of the final value within about the first minute. Spiro &

Selwood focused on caffeine rather than *TDS*, and they developed a three-phase model: diffusion of caffeine through the bean particle from center to surface, mass transfer across the solid liquid interface, and diffusion through the Nernst layer to the bulk (Spiro and Selwood, 1984). The model was based on Fick's Law of diffusion with an experimentally determined temperature-dependent partition coefficient at equilibrium. Their caffeine extraction experiments at various temperatures and grind sizes, under constant agitation, showed that the caffeine concentration rapidly increased near the beginning of extraction before plateauing, and that the internal diffusion of caffeine through the coffee particle is the rate limiting step (Spiro et al., 1989; Spiro and Page, 1984; Spiro and Selwood, 1984).

Later work by Zanoni et al. applied Spiro and Selwood's model to the extraction of extractable soluble substances in full immersion brewing under constant agitation at 90°C (Zanoni et al., 1992). They observed that the extraction involved what they referred to as a rapid "washing step" characterized by rapid dissolution of 85-90% of the soluble mass within the first minute. This rapid dissolution step was followed by a slower diffusion process that eventually yielded a final or equilibrium concentration. Other coffee extraction kinetics studies also reached similar conclusions, in that full immersion coffee extraction involves an almost instantaneous dissolution followed by slower diffusion (Moroney et al., 2016; Stapley, 2002). However, the distinction between the initial rapid phase and slower diffusion phase is ambiguous. Spiro et al. suggested that the rapid dissolution is governed by differences in diffusion of soluble constituents (Spiro, 1993), while Zanoni et al. characterized the first minute of brewing as "washing" (Zanoni et al., 1992); in the face of this complexity, Stapley suggested early stage extraction, where the brew concentration is below 35% of its final value, should be ignored since the true instantaneous dissolution for all solubles is hardly measurable (Stapley, 2002).

More sophisticated mathematical models have been recently developed to describe full immersion coffee extraction kinetics in a well-mixed system. Moroney et al. used a multiscale flow extraction model to predict full immersion coffee extraction as a limiting case of batch-wise brewing (Moroney et al., 2016, 2015); these models require solving sets of coupled differential equations numerically with multiple fitting parameters, which complicates interpretation of the parameters in practical industry scenarios. Wang and Lim found that *TDS* measurements are well fitted to a Weibull distribution model, a pseudo-first order model, and a pseudo-second order model (Wang and Lim, 2021); these simpler data-fitting models are decoupled from fundamental mass transfer principles, which makes incorporation of brewing parameters into the model challenging. Furthermore, most prior work focused on full immersion brewing with continuous agitation (Voilley and Simatos, 1979; Zanoni et al., 1992) or a form of shaking upon completion of the brew (Wang and Lim, 2021). In practice, full immersion brews are rarely agitated. French press, cold brew, and cupping all have minimal external agitation during the extraction. Thus, a simple but universal model is needed to capture and predict the extraction dynamics of full immersion brewed coffee in response to large range of brewing parameters for practical applications.

Here, we report data from a massive investigation of full immersion brewing dynamics, comprising more than 3,000 individual measurements of *TDS* versus time for a variety of different coffee preparation factors. Specifically, we (1) investigated the effects of roast level, brewing temperature, and post-harvest processing method from different origins, on the extraction dynamics of full immersion brewed coffee; and (2) interpreted the extraction dynamics using an updated diffusion-limited model. The main goal is to provide coffee practitioners with better insight on how to achieve desired *TDS* levels with full immersion brews.

The remainder of the paper is organized as follows. First, we review the theory for diffusion-limited caffeine extraction, and update it in the context of coffee solubles extraction applicable for practical full immersion coffee brewing. Then, we describe our experimental methodology, and then report the findings of the impact of coffee preparation factors on the extraction dynamics of full immersion brews and assess the validity of the proposed model. We finish by discussing the implications of our data for the coffee industry.

3-3. Theory

The main goal of this section is to elucidate the simplest mathematical description of the dynamics of full immersion coffee extraction. As discussed in our previous study (Liang et al., 2021), the mass of coffee grounds (M_g) and the mass of water (M_w) together define the brew ratio,

$$R_{brew} = \frac{M_w}{M_g}. \tag{3-1}$$

The brew ratio is an input parameter at the discretion of the brewer. There are two important quantitative output measures for every coffee brew, the TDS and E. The TDS is the mass fraction of solubles present in the consumable coffee beverage, and E is the fraction of solubles removed from the coffee grounds during the extraction with water. These two quantities are related via conservation of mass arguments (Liang et al., 2021) as

$$E = \frac{TDS}{1-TDS} R_{brew}. \tag{3-2}$$

Note that *E* is the theoretical prediction of the instantaneous extraction yield of the brew, not the extraction yield measured after drying spent coffee grounds in the oven; the oven-drying *E* tends to underestimate the actual *E* due to retained liquid trapped between the moist spent grounds (Liang et al., 2021). Because *TDS* is readily measured experimentally via refractometry, and Eq. (3-2) allows calculation of *E* from *TDS*, the main challenge is to determine a predictive equation for how *TDS* varies with time.

Here, we focus on a simple diffusion-limited model that follows first order kinetics to capture the extraction dynamics of full immersion brewed coffee. The full immersion coffee extraction equation is adapted from a three-phase mass transfer model of caffeine infusion (Spiro and Selwood, 1984), but as originally suggested by Zanoni et al., we apply it to all extractable coffee solubles in full immersion coffee brewing (Zanoni et al., 1992). In this approach, coffee grounds are modeled as spherical particles, and the extraction of coffee solubles involves 1) diffusion from the center of the coffee particle to the surface, 2) mass transfer across the solid-liquid interface, and 3) diffusion through the Nernst layer to the bulk of the coffee brew (Spiro and Selwood, 1984). Our goal is to streamline this model to the simplest form possible that accurately captures the dynamics of full-immersion extraction.

A first simplification is that we neglect the spatial concentration gradients that occur within the brew. Previous work established that non-agitated full immersion brews exhibit a pronounced vertical concentration gradient that inverts as the coffee grounds degas and sediment (Liang et al., 2023). In other words, the *TDS* is initially highest near the top of the brew, but then at later times the *TDS* is highest at the bottom of the brew. This observation means that even in the absence of external agitation, the brew undergoes a slow "natural agitation" due to the sedimentation of the coffee grounds. The data further indicated that samples drawn from the geometric center of the brew (i.e., outside of the "crust" of floating coffee grounds near the top or the layer of sedimented grounds at the bottom) provide *TDS* measurements that reflect the average *TDS* throughout the duration of the brew. Accordingly, despite the absence of external agitation we assume the coffee brew is well-mixed and that the instantaneous *TDS* of the brew can be characterized with a single average value.

Our other major simplifications are that we assume there is no accumulation at the solid/liquid interface of the individual coffee particulate, and that the concentration inside the wet coffee particulate rapidly reaches an effective equilibrium concentration. Thus, the difference between the equilibrium concentration inside the coffee ground and the instantaneous concentration of coffee solubles in the external brew provides the driving force for mass transfer. If we apply conservation of mass to a control volume that includes the liquid surrounding the coffee grounds, the rate of accumulation of soluble species in the liquid must equal the rate of mass transfer out of the coffee ground interiors, which we model as

$$\frac{dC}{dt} = k\left(C_{eq} - C\right). \tag{3-3}$$

Here C is the instantaneous concentration of the coffee solubles present in the liquid coffee brew (equivalent to the *TDS*), C_{eq} is the concentration of coffee solubles in both the wet coffee grounds and liquid coffee brew at equilibrium, and k is the effective mass transfer coefficient that subsumes all of the resistances to mass transfer into one lumped parameter.

As a first order differential equation, Eq. (3-3) requires an initial condition. As described above, much prior work has established the existence of a rapid dissolution process that occurs while the water is poured onto the coffee grounds, but we ignore those complicated dynamics and instead specify that there is an effective initial or “rinse” concentration that is obtained

$$C = C_0, \; t = 0 \tag{3-4}$$

where C_0 is the initial concentration. Although in practice it takes some finite amount of time for the water to pour onto and mix with the coffee grounds, this time is negligible compared to the longer extraction times of interest here (measured in minutes to days). Thus $t = 0$ is practically defined as the moment upon completion of water addition to the brew. (We use the phrase “rinse concentration” instead of “wash concentration” to avoid possible confusion with the “washed” method of post-harvest processing of green coffee beans.)

Integration of Eq. (3-3) and application of initial condition Eq. (3-4) yields the “universal” full immersion coffee extraction equation,

$$TDS = \left(C_{eq} - C_0\right)\left(1 - e^{-kt}\right) + C_0 \quad (3\text{-}5)$$

(cf. Fig. 3-1). This equation can then be used to calculate the instantaneous extraction via equation (3-2). The typical TDS of full immersion brewed coffee is between 1% to 4% for any brew ratio $R_{brew} \geq 5$ based on our previous study (Liang et al., 2021). Assuming the quantity of $(1 - TDS)$ is close to 1 such that $TDS \ll 1$, substitution of Eq. (3-3) in Eq. (3-4) yields the expression of the extraction equation in terms of E to a good approximation,

$$E = R_{brew}\left[\left(C_{eq} - C_0\right)\left(1 - e^{-kt}\right) + C_0\right]. \quad (3\text{-}6)$$

In addition, the estimated equilibrium constant, K, can be estimated from the equilibrium extraction yield, E_{eq}, using a prior desorption model (cf. Eq. (3-15) in Liang et al.'s study (Liang et al., 2021)),

$$E_{eq} = KE_{max}, \quad (3\text{-}7)$$

with a maximum extraction yield, E_{max}, which is typically around 30% (Moroney et al., 2015).

We emphasize that the full immersion coffee extraction model described here assumes that extraction of coffee solubles involves two important processes: (1) a rapid "rinsing" dissolution process that is established upon contact with water, followed by (2) a much slower diffusion process. A convenient way to characterize the relative magnitudes of these two processes is the "rinse ratio" defined as,

$$R_{rinse} = \frac{C_0}{C_{eq}}, \quad (3\text{-}8)$$

which by definition is bounded between 0 and 1.

Finally, we note that the mass transfer coefficient is related to an effective species-averaged diffusivity. Assuming diffusion through the interior of the coffee particle is the rate-limited step for all coffee solubles, then an effective diffusivity through the coffee particle D, of all extractable coffee solubles from the brew can be estimated using the equation (Jaganyi and Madlala, 2000; Spiro, 1993; Spiro and Selwood, 1984; Zanoni et al., 1992)

$$D = \frac{kr^2}{12}, \tag{3-9}$$

where r is the radius of the coffee particles.

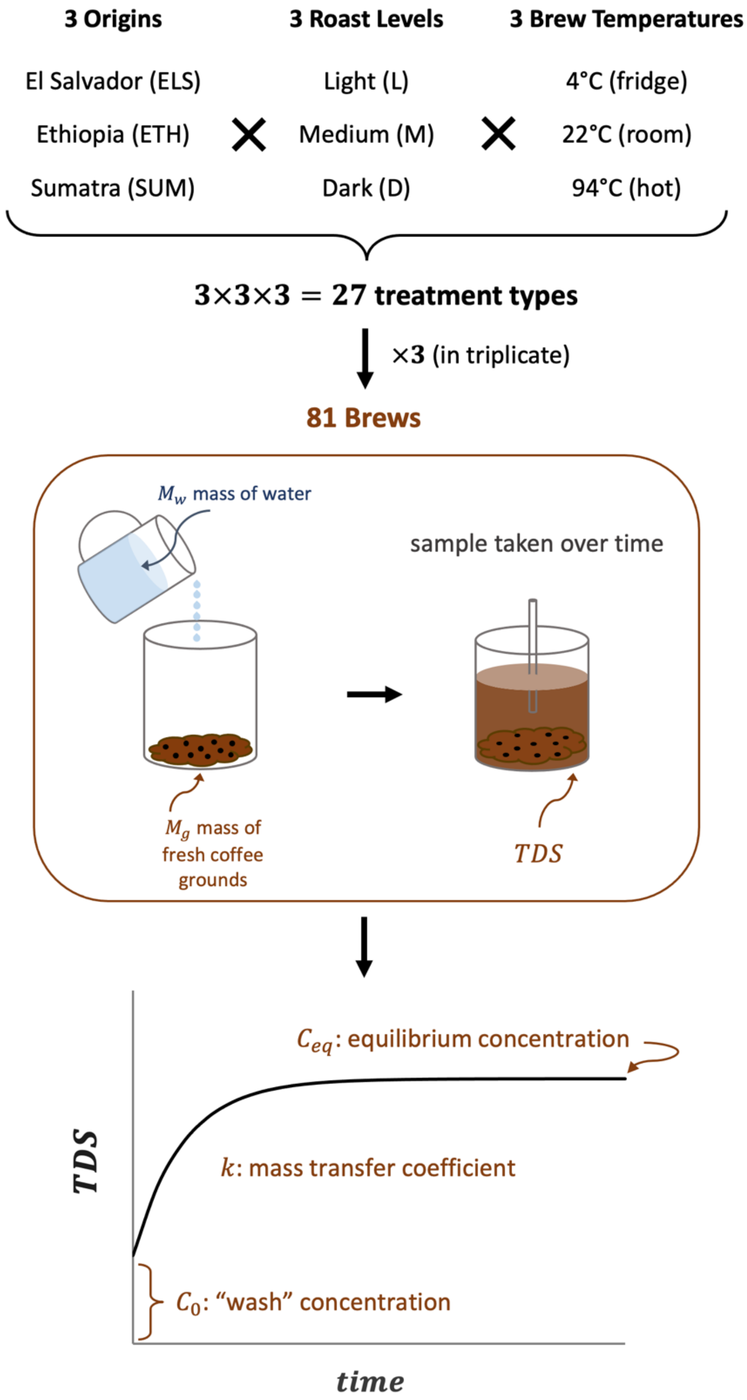


Figure 3-1. Top: overview of the experimental design. Middle: definition sketch of the brewing experiments. Bottom: qualitative sketch of the "universal brewing curve" for the *TDS* versus time.

3-4. Experimental Methodology

3-4.1 Overview of the Experimental Design

The main goal of the experiments was to assess whether Eq. 3-5 truly serves as a "universal curve" for full immersion coffee brewing across a variety of different brewing conditions. Accordingly, a 3x3x3 factorial experimental design was used to study the effects of origin, roast level, and brewing temperature on the extraction dynamics of full immersion coffee (cf. Fig. 3-1). Green coffees from three different origins (all post-harvest processed differently) were each roasted to three different roast levels, and then each roasted coffee was brewed using full immersion at three different temperatures. This experimental design yielded 27 treatment types, each of which was repeated in triplicate. Each individual brew was sampled at designated timepoints throughout the entire brewing period to obtain quantitative measurements of the *TDS* versus time, as described in detail below.

3-4.2 Coffee

Three different types of Coffea arabica green coffee beans from three different origins with different processing methods were used: honey processed El Salvador Cerro Las Ranas (ELS), washed processed Ethiopia Guji organic (ETH), and wet-hulled processed Sumatra Fair-Trade Organic Takengon (SUM). In all of these three processing methods, the coffee cherries were depulped shortly after harvest to remove the outer skins and pulps. The key difference lies in treatment with mucilage layer: the so-called "honey process" retains mucilage for spontaneous fermentation while drying, while the washed and wet-hulled processes completely remove it via fermentation while submerged in water (De Bruyn et al., 2017). After that, washed processing involves a drying step before parchment removal (hulling) (Rotta et al., 2021). In contrast, wet-hulled coffee is only partially dried before hulling, so the seed is fully exposed without the protective parchment while drying (Hoffmann, 2018). These three coffees were chosen because qualitatively they have dramatically different flavor profiles (Batali et al., 2022).

Each green coffee was roasted to three different roast levels: light (L), medium (M), and dark (D). All roasts were performed at the UC Davis Coffee Center on a single day using a Probat P-5 drum roaster (Probat-Werkevon Gimborn Maschinenfabrik GmbH, Emmerich am Rhein, Germany). The color of the roasted coffee was measured using an Agtron Analyzer (cf. Supplementary Table 3-S1), gauged by the Agtron Gourmet Color Scale published by the SCA (Specialty Coffee Association, 2018). The average Agtron scores for the roasted coffee beans were 57, 49, and 37 for light, medium, and dark roast, respectively. The roasted coffees were allowed to rest at room temperature for a week after roasting to degas, and then vacuum-sealed in bags and stored in a freezer at −20 °C to maintain consistency in coffee bean quality against storage or aging effects (Cotter and Hopfer, 2018). Before use, each individual bag of coffee was defrosted overnight to room temperature.

3-4.3 Brewing procedure

All roasted coffees were ground immediately prior to brewing using a medium grind size on a Mahlkönig Guatemala Lab Grinder (Mahlkönig USA, Durham, NC, USA) with a median particle size of $972 \pm 19\ \mu m$ (Liang et al., 2021). Ground coffee was brewed using water at three different temperatures: 4°C (typical refrigerator temperature), 22°C (room temperature), or 94°C (within the range of hot brewed coffee suggested temperature (Lingle, 2011)). Nestlé Pure Life Purified Water was used for all brews (Nestlé Waters North America, Inc., 2021). For the fridge temperature brews, water was pre-refrigerated to 4°C; for the room temperature brews, water was controlled at 22°C; for the hot brews, water was heated to a 94°C using an OXO Adjustable Temperature Pour-Over Kettle (OXO, New York City, NY, USA).

All coffees were brewed using a full immersion brewing technique in a 1-L glass beaker at a water-to-coffee brew ratio $R_{brew} = 5$, which a typical brew ratio for cold brew concentrate used in the industry (Toddy, 2020). First, 120 g of coffee grounds were measured and placed into the beaker. Then, 600 g of water at a target temperature (4, 22, or 94°C) was poured into the beaker using the same OXO Pour-Over Kettle. A circular pouring motion was used to ensure all the coffee grounds were fully wet. As a consistency check, this "pour-in" time was measured starting from the moment of coffee grounds upon contact with water until the beaker contents reached the designated brew ratio. The timing of the brew ($t = 0$) started upon completion of the water pouring. The fridge brews were brewed for 54 hours, the room-temperature brews were brewed for 46 hours, and the hot brews were brewed for 3 hours. During brewing, the fridge brews were stored in a refrigerator at 4°C, while the room and hot brews were sat on a wooden countertop with no lid at room temperature. This procedure was chosen for fidelity with brewing processes widely used in industry, where hot brews are very rarely stored in constant temperature baths. We emphasize that the hot brews decreased in temperature with time, while the fridge and room temperature brews remained roughly constant at their specified temperatures.

3-4.4 TDS Measurements

Throughout the entire brewing process, small individual samples (approximately 0.5 mL per sample) were collected using a disposable pipet from the middle of the coffee brew at designated time points. Besides this gentle sampling, no stirring or intentional agitation was conducted in any format aside from the naturally occurring mixing due to the off-gassing and sedimentation of the coffee grounds (Liang et al., 2023). For the fridge brews, individual samples were collected at 0, 1, 5, 15, 30 minutes, then every 30 minutes from 0.5 to 8 hours, then every hour from 8 to 14 hours, then every 2 hours from 14 to 24 hours, and finally at 28, 32, 38, 46, and 54 hours (yielding a total of 36 samples per fridge brew). For the room temperature brews, samples were collected at 0, 1, 3, 5, 15, 30 minutes, then every 30 minutes from 0.5 to 8 hours, then every hour from 8 to 14 hours, then every 2 hours from 14 to 30 hours, another sample at 36 hours, and finally three samples were drawn at 46 hours, with two drawn from the periphery and one from the center of the brew to assess spatial uniformity (yielding a total of 39 samples per room-temperature brew). For the hot brews, samples were obtained every 30 seconds from 0 to 1 minutes, every minute from 1 to 14 minutes, every 2 minutes from 14 to 20 minutes, every 5 minutes from 20 to 45 minutes, every 15 minutes from 45 to 90 minutes, and every 30 minutes thereafter until the end of 180 minutes (yielding a total 30 samples per hot brew). Each brew was performed with three trial replicates.

Because a brew ratio of $R_{brew} = 5$ is unusually strong for typical hot brews, we also investigated an additional brew ratio $R_{brew} = 15$ (comprising 900 g water and 60 g coffee grounds) using 94°C water, otherwise following the same procedures. This brew ratio is more typical for hot brews, e.g., in a French press or for cupping (Specialty Coffee Association, n.d.). Again, all measurements were performed with three trial replicates.

After each sample was collected, it was immediately centrifuged using a Thermo Fisher Scientific mySPIN 6 mini centrifuge (Thermo Fisher Scientific, Waltham, MA, USA) at 6000 RPM for 2 minutes to separate liquid brew from undissolved particles. Once the centrifuged sample reached room temperature (typically within a few minutes for the hot or fridge brews), a drop of the supernatant (approximately 0.25 mL) of the centrifuged liquid sample was then placed in a digital refractometer (VST, Inc) to measure the *TDS*. The *TDS* refractometer was calibrated using the method specified in the "digital refractometer calibration" section of previous work (Liang et al., 2021). Given the above sampling schedules and the 27 sample types each measured in triplicate, a total of 3,420 *TDS* measurements were collected during this study.

3-4.4 Data and statistical Analysis

Data analysis was conducted using RStudio 2022.07.1 Build 554 (Posit, PBC, Boston, MA) and MATLAB R2020b (The MathWorks, Inc., Natick, MA). Non-linear regression of *TDS* to brew time via Eq. (3-5) was performed using the MATLAB built-in function *lsqcurvefit*, where k, C_0, and C_{eq} served as the fitting parameters. The corresponding best-fit parameters were evaluated MATLAB built-in function *nlparci* to return a 95% confidence interval. The adjusted R^2 value of the regression was extracted from MATLAB using the built-in function *fitnlm*, and the p-value was calculated using the MATLAB built-in function *coeftest*. Analysis of Variance (ANOVA) for each of the fitting parameters was conducted at 5% significance level using the R built-in function *aov*, where Origin, Roast, and Brewing Temperatures were the factors. All plots were generated using MATLAB R2020b.

3-5. Results

3-5.1 Dynamic TDS and E over Time

Our dynamic experiments shows that the *TDS* of non-externally agitated full immersion brews follows the “universal” curve regardless of brew temperature or coffee characteristics (Fig. 3-2). The *TDS* of all $R_{brew} = 5$ brews increased with brew time and plateaued to 3.4-4.5% for all origins, roast levels, and brew temperatures (Fig. 3-2A,B,C), and plateaued to 1.2-1.5% for the $R_{brew} = 15$ hot brews (Fig. 3-2D). Likewise, the corresponding extraction yields exhibited similar trends with an initially fast increase followed by a plateau in all trials tested (cf. Supplementary Fig. 3-3). Although all brews followed the same trends, there were quantitative differences in the dynamics observed with different brewing conditions. First, the final *TDS* of hot and room brews were greater than 4%, while the final *TDS* of fridge brews remained under 4%. The most rapid increase of *TDS* happened within the first 10 hours for the 4°C and 22°C brews, and within the first 30 minutes for the 94°C brews. Furthermore, the effect of roast level is more pronounced compared to the effect of origin. Particularly, the distinction among the dynamic *TDS* of coffee brews with light, medium, and dark roasts within a single origin is obvious, whereas the variability in the dynamic *TDS* across different origins is less clear. For example, Figure3- 1B shows that the dynamic *TDS* measurements of light, medium, and dark roasts of Sumatra (light green circles, green triangles, and dark green squares, respectively) are more distinct than any of the origins at a given roast level. Similar trends about the dynamic *TDS* measurements were also observed in the 22°C and the 94°C brews.

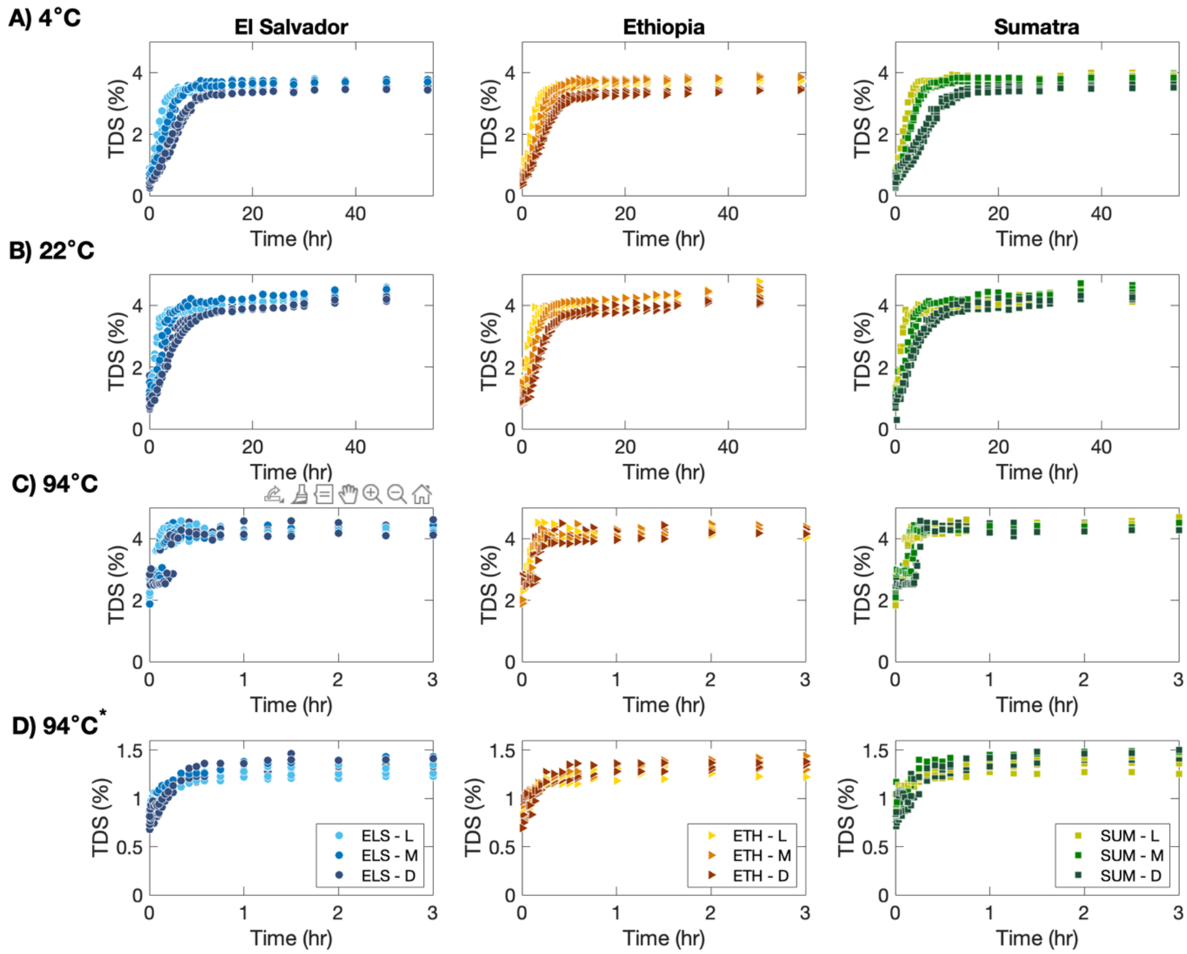


Figure 3-2. Experimental measurements of the *TDS* versus time for full immersion brews brewed at **A)** 4°C at $R_{brew} = 5$, **B)** 22°C at $R_{brew} = 5$, **C)** 94°C at $R_{brew} = 5$, and **D)** 94°C at $R_{brew} = 15$ (denoted with an asterisk). Different origins are denoted with different color schemes (blue for El Salvador, red for Ethiopia, and green for Sumatra), and different roast levels are denoted with different shapes (circles for light roast, triangles for medium roast, and squares for dark roast).

One subtle but noteworthy difference is that a sudden increase of *TDS* was observed in the hot $R_{brew} = 5$ brews around 4-15 minutes, and was most pronounced with the lighter roasts (Fig. 3-2C). This type of sudden *TDS* increase phenomenon was not observed in the 4°C or 22°C brews, nor in the 94°C brews at a more diluted $R_{brew} = 15$. The sudden increase appears to result from a rapid "collapse" and sedimentation of the thick crust of coffee grounds initially floating near the top of the brew; the sudden increase in *TDS* was concurrent with the sinking of a large fraction of the grounds. This sudden sinking presumably mixed the brew rapidly and increased the *TDS* when sampled from the middle of the brew (Liang et al., 2023). In contrast, the sedimentation of coffee grounds in the 4°C, 22°C, or the 94°C $R_{brew} = 15$ brews happened more slowly and gradually throughout entire the course of brewing.

3-5.2 Assessment of the Universal Brewing Curve

Our results indicated that the extraction dynamics of full immersion coffee brews are qualitatively captured by the proposed coffee extraction model equation (Eq. (3-5)). Nonlinear regression of the data against the model prediction yielded excellent quantitative agreement, as shown in Figure 3-3 and Supplementary Figures 3-S2A, 2B, and 2C. With only three fitting parameters from the model, (C_{eq}, C_0, and k), the characteristics of any extraction dynamics at various brewing conditions, including origin, roast level, brew temperature and brew ratio are well described by the universal curve. In addition, for 4°C, 22°C, and 94°C brews at $R_{brew} = 5$, nonlinear regressions of the individual trials measured *TDS* over time data to Eq. (3-5) shows that yields an average p-value in the order of 10^{-24} and adjusted R^2 value of 0.945, indicating an excellent fit of the model to the experimental data. Similar results about the goodness of fit were also obtained from the 94°C trials at $R_{brew} = 15$, with an average p-value in the order of 10^{-28} and adjusted R^2 value of 0.954, again strongly corroborating the hypothesis that full immersion extraction dynamics are well represented by the universal brewing curve.

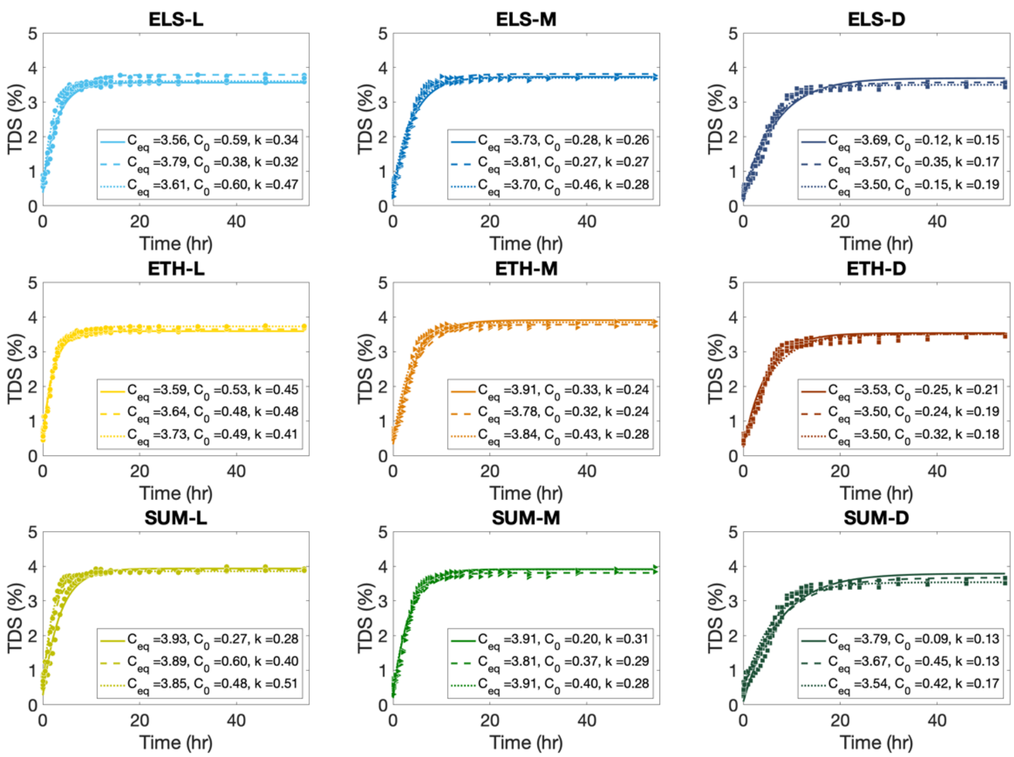


Figure 3-3. Experimental measurements of the *TDS* versus time with the best fit universal brewing curve (Eq. 3-5, solid lines). Each graph shows three trial replicates (markers) and corresponding best fits(solid or, dashed, or dotted lines). All graphs are at $R_{brew} = 5$ and brewed at 4°C (fridge). See also supplementary figures 2A, 2B, and 2C for data at other temperatures and brew ratios.

3-5.3 Effects of Origin, Roast Level, and Brew Temperature on the Extraction Dynamics

With the universal brewing curve, a convenient way of comparing the extraction dynamics is by comparing the quantitative values of C_{eq}, C_0, and k for different origins, roast levels, and brew temperatures. Boxplots of the regressed values of C_{eq}, C_0, and k for all of the individual trials are shown in Figure 3-4, where different brewing conditions are arranged by columns. Overall, brewing temperature had the largest impact, while the effects of roast level and origin varied in magnitude. Both the equilibrium concentrations C_{eq} and the initial rinse concentrations C_0 are dominated by the brewing temperatures. Furthermore, the ANOVA results of C_{eq}, C_0, and k at $R_{brew} = 5$ shows that the effect of brew temperature and roast Level are significant for all three parameters, while the effect of origin is only significant for C_{eq} and k (cf. Supplementary Table 3-S2).

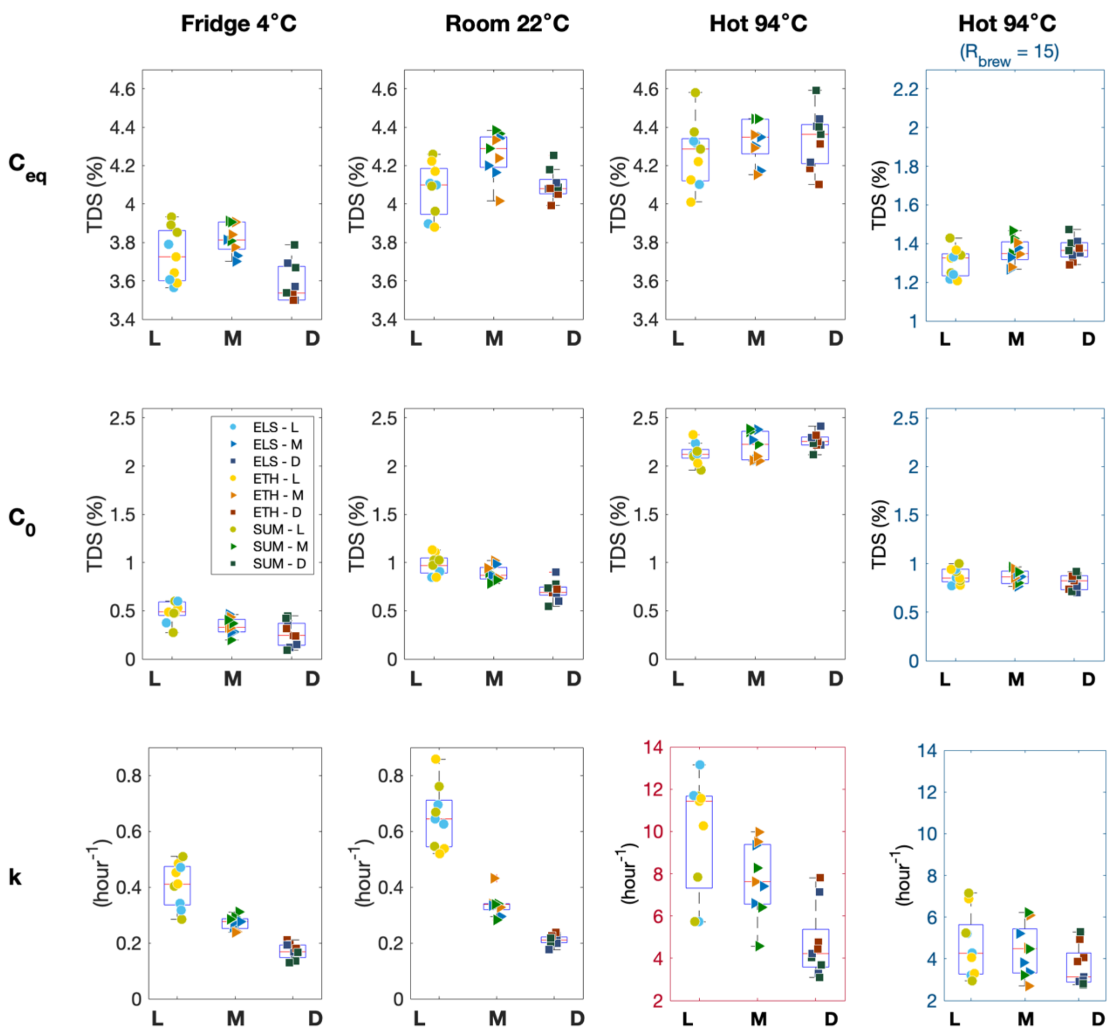


Figure 3-4. Boxplots of the regressed values of the three fitting parameters C_{eq} (top row), C_0 (middle row), and k (bottom row). Each marker represents an individual trial replicate. of full immersion brews using coffee from 3 origins (ELS, ETH, SUM), 3 roast levels (L, M, D), and brewed at 3 temperatures (Fridge 4°C, Room 22°C, Hot 94°C) at $R_{brew} = 5$, and 94°C at $R_{brew} = 15$ denoted in blue. The regressed values equilibrium concentration (C_{eq}), initial concentration (C_0), and effective mass transfer coefficient (k) serve as the fitting parameters to the model equation $TDS = \left(C_{eq} - C_0\right)(1 - e^{-kt}) + C_0$. The vertical axes for $R_{brew} = 5$ are consistent across temperatures at a given fitting parameter, except for k at 94°C in red. The vertical axes for $R_{brew} = 15$ are in blue. Established significance at 5% from ANOVA of the effects of coffee preparation factors on fitting parameters at $R_{brew} = 5$ are specified in Supplementary Table 2.

At $R_{brew} = 5$, across roast levels and origins, C_{eq} significantly increases with brewing temperature, with average values of $3.71 \pm 0.14\%$, $4.14 \pm 0.14\%$, $4.31 \pm 0.14\%$, for fridge, room, and hot brews, respectively (top row, Fig. 3-4). The effects of both origins and roast on C_{eq} are much smaller than temperature indicated by the larger p-values (cf. Supplementary Table 3-S2). For the $R_{brew} = 15$ hot brews, as expected the final concentration was more diluted with an average C_{eq} is $1.34 \pm 0.07\%$, with non-significant roast or origin effects. Furthermore, the equilibrium *E* remains stable at $21.14 \pm 1.57\%$ for all the $R_{brew} = 5$ brews at various brewing conditions. In fact, the estimated equilibrium constant, *K*, from equilibrium *E* using a prior desorption model (cf. Eq. (3-7)) assuming a maximum extraction yield of 30%, falls within 0.705 ± 0.052 (cf. Table 3-1). This value accords with the prior measured value of 0.717 ± 0.007 (Liang et al., 2021).

Temperature	Roast Level	k (10^{-4} s^{-1})	D (10^{-12} m^2/s)	K
4°C	Light	1.134 ± 0.0766	2.232 ± 1.725	0.646 ± 0.025
	Medium	0.758 ± 0.219	1.491 ± 0.530	0.662 ± 0.014
	Dark	0.472 ± 0.0673	0.930 ± 0.603	0.620 ± 0.019
22°C	Light	1.807 ± 0.308	3.556 ± 2.422	0.708 ± 0.025
	Medium	0.934 ± 0.115	1.839 ± 0.906	0.741 ± 0.022
	Dark	0.585 ± 0.0495	1.151 ± 0.390	0.712 ± 0.014
94°C	Light	27.48 ± 7.67	54.09 ± 60.42	0.742 ± 0.031
	Medium	21.52 ± 4.84	42.36 ± 38.07	0.754 ± 0.020
	Dark	13.11 ± 4.605	25.80 ± 36.26	0.755 ± 0.027

Table 3-1. The effective mass transfer coefficient, estimated diffusivity, and estimated equilibrium constant averaged across origins and trial replicates for different brewing temperatures and roast levels at $R_{brew} = 5$.

The rinse concentration C_0 increases much more dramatically with brewing temperature, with averages of $0.37 \pm 0.14\%$, $0.86 \pm 0.15\%$, and $2.20 \pm 0.12\%$, for the 4°C, 22°C, and 94°C brews, respectively, at $R_{brew} = 5$ (second row, Fig. 3-4). In comparison between the hot brews, the average C_0 of $R_{brew} = 15$ hot brews is $0.85 \pm 0.08\%$ regardless of roast or origin, which is smaller than half of the rinse concentration of $R_{brew} = 5$ brews. Thus, the initial *TDS* of full immersion brews highly depend on both temperature and brew ratio.

Most importantly, the extractions rates of full immersion brews under different experimental factors are captured by the effective mass transfer coefficient k from the model equation. Unsurprisingly, the extraction rate was highly dominated by brewing temperature. In fact, the effect of temperature is shown by the huge difference in scale, in which k is approximately 20 times higher in the 94°C brews than the 4°C or 22°C brews averaged across roast and origin for the $R_{brew} = 5$ brews (Fig. 3-4). Furthermore, roast level also has an important effect on the extraction rate of full immersion brews, while the effect of origin is minimal. At a given brewing temperature, the coffee brewed with light roast coffee extract the fastest indicated by the highest k value, and the brews with dark roast coffee extract the slowest (cf. Table 3-1). Specifically, light roast extract nearly 3 times faster than dark roast at 4°C and 22°C, and two times faster than dark roast at 94°C. In other words, it takes longer for the dark roasted coffee to reach equilibrium *TDS*, and this effect is more pronounced in the room and fridge brews. Conversely, neither the effect of roast level or origin on any of the fitting parameters of hot brews at $R_{brew} = 15$ is significant (cf. Supplementary Fig. 3-S4), suggesting the extraction dynamics of a more diluted brew at high brewing temperatures does not depend on origin or roast level of coffee bean used.

3-5.4 The Rinse Ratio

The rinse ratio characterizes the relative contribution of the rapid dissolution during the initial contact with the water to the overall extraction process. A boxplot of the rinse ratio R_{rinse} of all individual trial replicates at various brewing temperatures is shown in Figure 3-S5. Regardless of origin and roast level, R_{rinse} increased with brewing temperature. At $R_{brew} = 5$, the 94°C brews reached an average R_{rinse} of 0.511 ± 0.033, while the 22°C and 4°C brews reached 0.207 ± 0.037 and 0.099 ± 0.039, respectively. In other words, more than half of the soluble material immediately dissolved into solution upon contact with hot water, while only 20% and 10% rapidly dissolved for the room temperature and cold brews, respectively. Furthermore, the average R_{rinse} of the 94°C brews at the higher brew ratio $R_{brew} = 15$ was 0.632 ± 0.05, which is significantly higher than for the more concentrated $R_{brew} = 5$ hot brews. In addition to the difference caused by brew ratio, the "pour-in" time might have also contributed for the difference in R_{rinse}. The average measured "pour-in" times were 21.0 ± 1.8 s dispensing 600 g water for all the $R_{brew} = 5$ brews, and 30.5 ± 1.9 s dispensing 900g water for the $R_{brew} = 15$ brews. Presumably under a similar water "pour-in" rate, more solubles were rapidly rinsed from the coffee grounds due to the longer contact time with water until the brew reached the desired brew ratio.

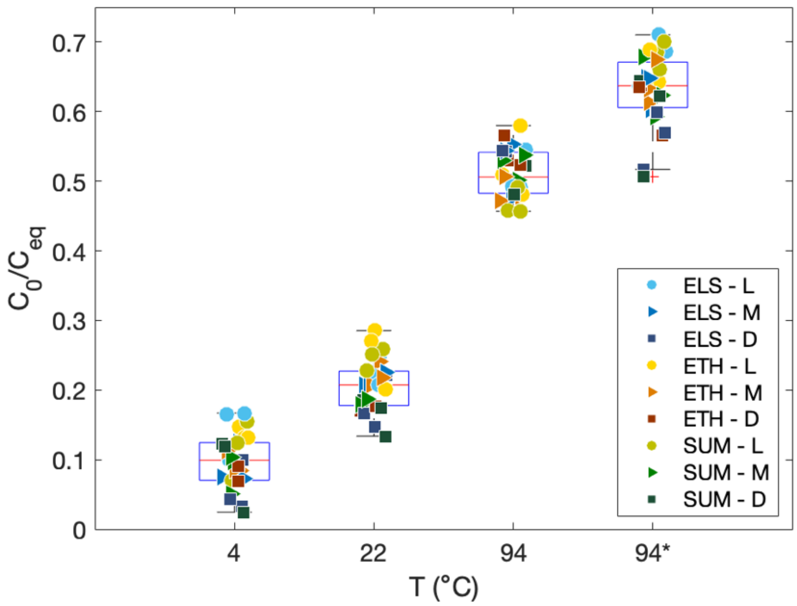


Figure 3-5. Boxplot of the "rinse ratio" $R_{rinse} = \frac{C_0}{C_{eq}}$ at various brewing temperatures of individual trial replicates of full immersion brews at $R_{brew} = 5$, and $R_{brew} = 15$ brews denoted in asterisk.

3-6. Discussion and Conclusions

The overarching conclusion from this study is that the "universal brewing curve" works for a wide variety of full-immersion brewing conditions. Specifically, our observations strongly corroborate the general finding that the coffee extraction process involves a rapid dissolution step followed by a slow diffusion step until reaching a final equilibrium value, in accord with previous studies of full immersion brewing (Moroney et al., 2016; Zanoni et al., 1992). Our data reported here further shows that the dynamic *TDS* and extraction of full immersion brews over a wide range of coffee preparation parameters including origin, roast level, brewing temperature, and brew ratio can be characterized, compared, and predicted using an updated and extended diffusion-limited mass transfer model with the three key parameters C_{eq}, C_0, and k. We validated this model with an extensive set of experimental data, comprising 3,420 *TDS* measurements. Brewing temperature most strongly impacted the extraction dynamics as expected; most interestingly, roast level was also found to significantly affect the extraction rate, in which the darker roasts extract slower than lighter roasts.

3-6.1 Lighters Roast Extracts Faster Than Darker Roasts

One of the most interesting findings of this study is that darker roast extracts slower with this effect being the most pronounced at low brew ratio and low brewing temperature. The composition of soluble coffee compounds is extremely complex, and coffee roasting contributes largely to the reaction and formation of these flavor compounds, resulting different composition of extractable coffee solubles at different roast level (Rostagno et al., 2015; Rufián-Henares and Pastoriza, 2015; Sunarharum et al., 2014; Tian et al., 2018; Wei and Tanokura, 2015; Yeager et al., 2021). As one of the major components of coffee beverage, the amount of melanoidins, increases with the severity of roasting in considering both time and intensity of the thermal treatment (Bekedam et al., 2008; Borrelli et al., 2002; Rufián-Henares and Pastoriza, 2015; Wei and Tanokura, 2015). A possible explanation of the slower extraction rate and lower diffusivity in darker roast is due to the accumulation of high molecular weight melanoidins as roasting proceeds. In addition to the difference in chemical composition between roast levels, other confounding factors of the coffee beans, such as porosity and density (Nakilcioğlu-Taş and Ötleş, 2019; Ortolá et al., 1998; Schenker et al., 2000), may also contribute to the difference in overall observed extraction kinetics.

3-6.2 The Parameters in the Full Immersion Coffee Extraction Model

Previous studies work by (Liang et al., 2021) found that the equilibrium *TDS* can be precisely controlled via the brew ratio and is relatively insensitive to roast level, grind size, and brewing temperature, at least over the narrow hot temperature range of 80 to 99°C . Over a larger range of coffee brewing temperatures, from 4 to 94°C, our data make clear that the equilibrium *TDS* and *E* are slightly lowered by about 12 percent in fridge brews compared to hot brews, but the equilibrium *TDS* and *E* for room temperature brew is the same as hot brew. In terms of maximizing extraction, this result suggests that room-temperature brews yield as much as hot brew, albeit more slowly.

Secondly, the initial rinse concentration is another important property that characterizes the full immersion coffee extraction. It has been ambiguous about how to distinguish between the dissolution and diffusion because these two processes happen congruently when considering all extractable coffee solubles together, as different soluble constituents with different solubilities and different diffusivities emerge at different rates (Spiro, 1993). It was suggested that experimental measurements below $R_{rinse} < 0.35$ in the beginning of the brew should be ignored in modelling the kinetics of coffee infusion due to inadequate sampling frequency (Stapley, 2002). However, the practical application of the extraction model should also be considered. Since full immersion coffee brewing in real-life setting generally involves adding water to a measured amount of coffee grounds to ensure coffee grounds are full wetted (Hoffmann, 2018; Lingle and Menon, 2017; Specialty Coffee Association, n.d.), our results imply that, practically, the "rinse" concentration can be conveniently defined as "the concentration of solubles extracted upon contact with water by the time the pouring is completed". In addition to water temperature, the rinse concentration can be potentially affected by a number of brewing parameters including grind size, brew ratio, water flow rate, water pouring motion, water pressure upon contact with coffee grounds, etc.

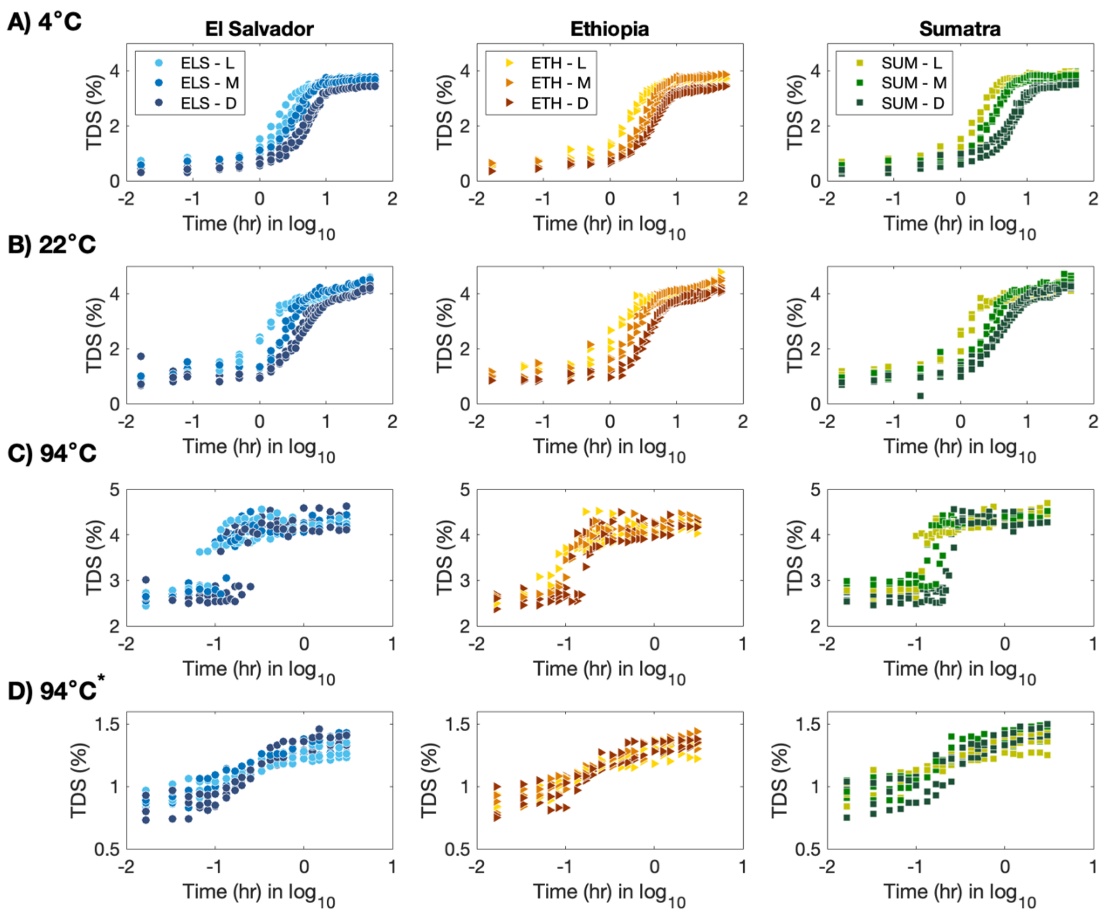
Third, the rate of extraction of full immersion coffee is expressed in k: an experimentally observed effective mass transfer coefficient that captures the mass transfer behavior of all coffee solubles including diffusion through coffee particle, mass transfer across surface, diffusion through the solution (Spiro and Selwood, 1984; Zanoni et al., 1992). Our results indicate that the rate of extraction of full immersion brew depends on both brewing temperature and roast level as shown in the Arrhenius plot (cf. Supplementary Fig. 3-S5). Furthermore, the effective diffusivity, $D,$ of all extractable coffee solubles from the brew can be estimated using Eq. (3-9) with a radius of 486μm (median particle size: 972±19 μm), the average effective diffusivities through coffee particle at 4°C, 22°C, and 94°C are 1.55×10^{-12} m^2/s, 2.18×10^{-12} m^2/s, and 4.08×10^{-11}m^2/s, respectively. This estimated value at 94°C is relatively faster compared to recorded values at 90°C (Spiro, 1993; Zanoni et al., 1992), however, it should be noted that prior estimations were based on extraction yield measured using an oven drying method, which underestimates the true extraction yield (Liang et al., 2021). As references, the effective diffusivities of caffeine and other mineral ions in different types of coffee at 80°C are in the order of 10^{-10} to 10^{-11} m^2/s (Jaganyi and Madlala, 2000), which accords with our estimated values. In addition, since lighter roast extracts faster than darker roasts, the effective diffusivities of coffee solubles at a fixed temperature are also estimated to decrease with roast level (cf. Table 3-1).

3-6.3 Practical Implications for Coffee Practitioners

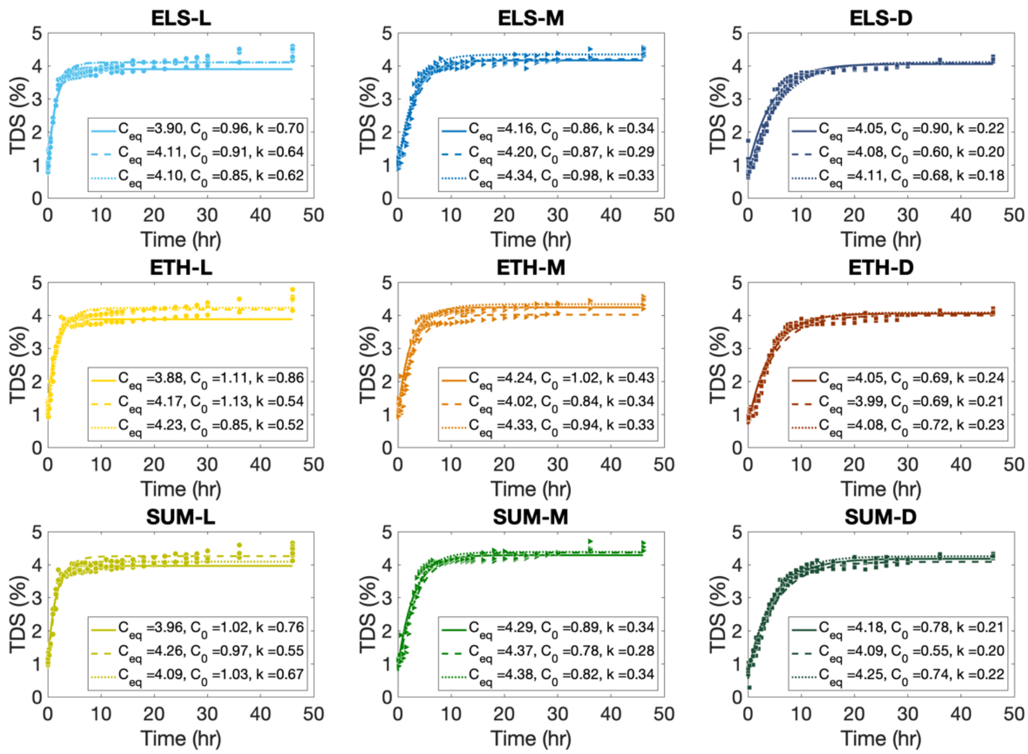
In terms of practical implications, the merit of simplicity and robustness of full immersion brewing technique is corroborated by our results. The final *TDS* and *E* of full immersion brews are primarily defined by the brew ratio and brew temperature; roast level of the coffee does not alter the equilibrium, but it only effects the rate of extraction, especially at fridge or room brewing temperatures. Thus, the achievable *TDS* and *E* of full immersion brews is a region majorly defined by the brew ratio and brew temperature as brew time proceeds, while the effect of origin is minimal, and roast level contributes mainly in terms of the path to get to a precise final *TDS* and E. We emphasize that this study was conducted with non-externally agitated full immersion coffee brews. There are other brewing factors in full immersion brewing that can potentially affect the extraction of coffee solubles including grind size, agitation, natural sedimentation and swelling of the coffee grounds, etc. (Cordoba et al., 2019; Fuller and Rao, 2017; Liang et al., 2023, 2021; Spiro and Page, 1984; Spiro and Selwood, 1984; Voilley and Simatos, 1979; Wang and Lim, 2021).

Furthermore, our parallel sensory study investigated the overall flavor profile of full immersion brewed coffee under a controlled *TDS* and temperature: it was found that roast level has the biggest effects compared to brewing temperatures and coffee origins, and there were also strong interaction effects between roast level and origin (Batali et al., 2022). However, the role of brew time contributed to the difference in dynamic *TDS* during the brewing, which subsequently effects the flavor perception remains unanswered. Our work here provides a basic understanding that brewing coffee from different roast levels to identical extraction times, especially under low temperature and low brew ratio, introduces a confounding factor of natural difference in *TDS* into the comparison. Thus, practitioners need to be aware that there are different coffee preparation factors that drive the difference in the physical properties and sensory perceptions of full immersion brewed coffee.

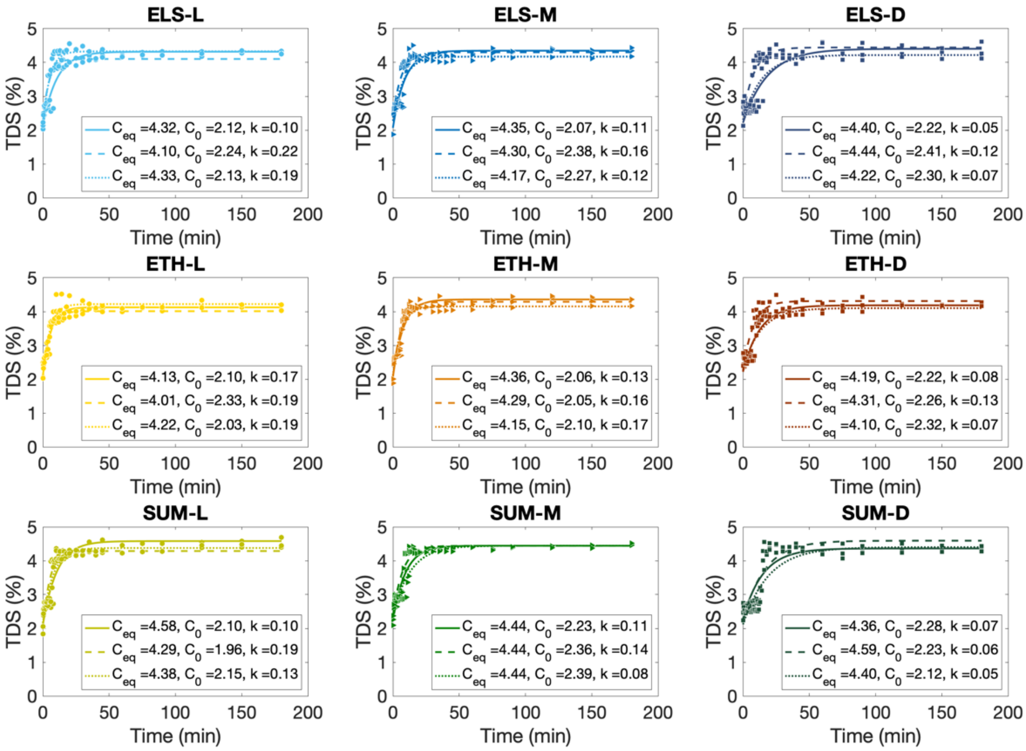
Supplementary Materials



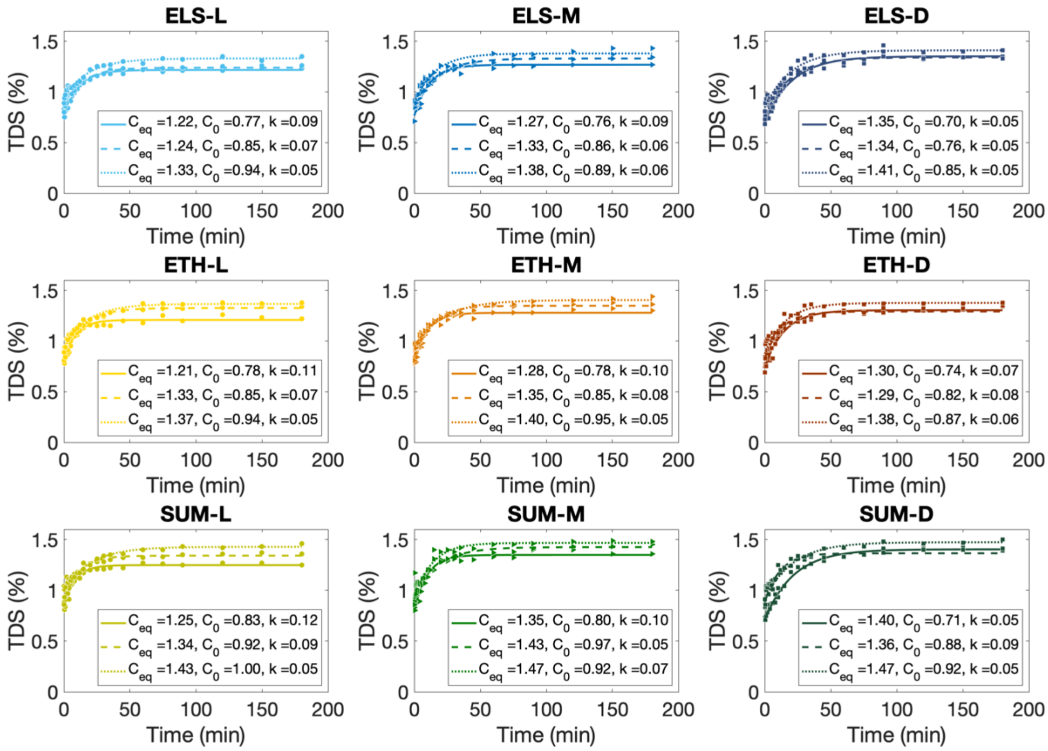
Supplementary Figure 3-S1. Scatter plots of dynamic *TDS* over $\log_{10}$ of time of full immersion brews using three differently processed coffee from different origins each roasted to three roast levels and brewed at **A)** 4°C at $R_{brew} = 5$, **B)** 22°C at $R_{brew} = 5$, **C)** 94°C at $R_{brew} = 5$, and **D)** 94°C brews at $R_{brew} = 15$ denoted with asterisk. Different origins are in different color schemes (blue for El Salvador, red for Ethiopia, and green for Sumatra), and different roast levels are in different shapes (circles for light roast, triangles for medium roast, and squares for dark roasts).



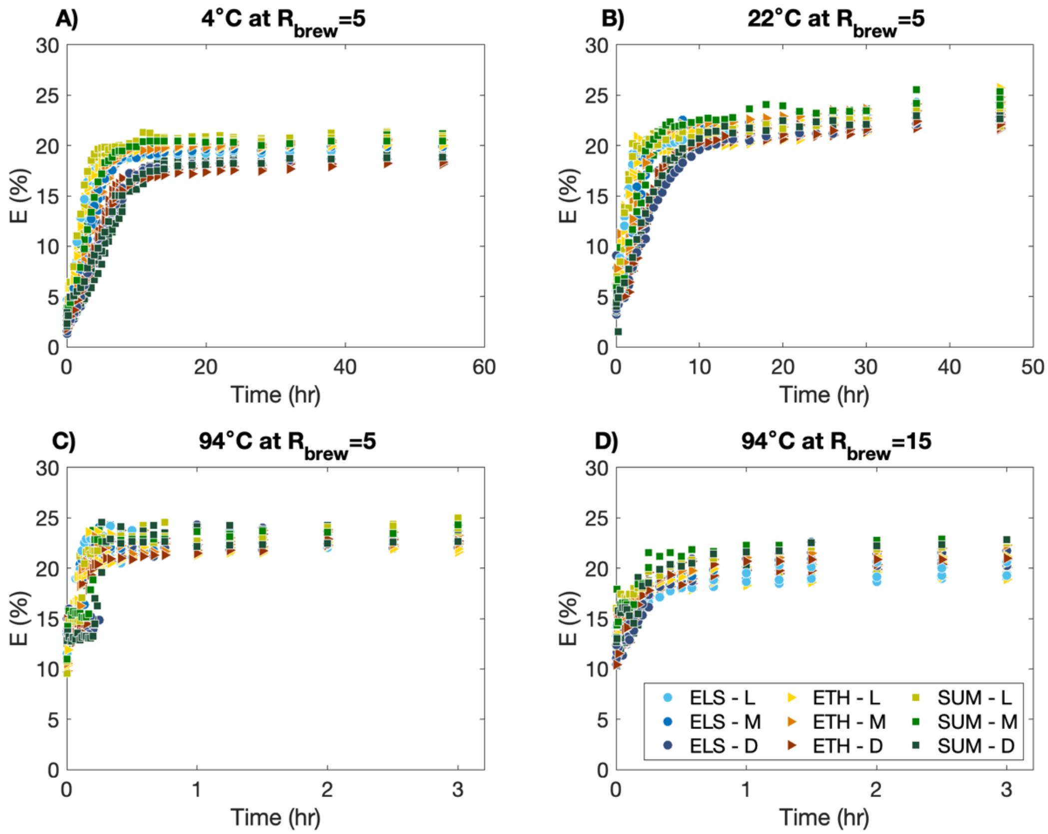
Supplementary Figure 3-S2A. Scatter plots of dynamic *TDS* over time of full immersion brewed coffee at $R_{brew} = 5$ of three origins at three roast levels brewed at 22°C (room). Individual trial replicate regressions to the model equation $TDS = \left(C_{eq} - C_0\right)\left(1 - e^{-kt}\right) + C_0$ are indicated by lines.



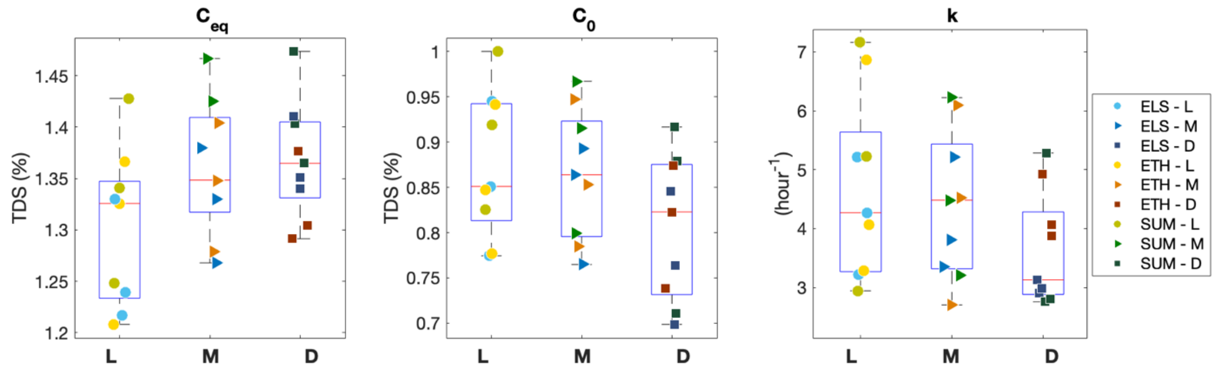
Supplementary Figure 3-S2B. Scatter plots of dynamic *TDS* over time of full immersion brewed coffee at $R_{brew} = 5$ of three origins at three roast levels brewed at 94°C (hot). Individual trial replicate regressions to the model equation $TDS = (C_{eq} - C_0)(1 - e^{-kt}) + C_0$ are indicated by lines; noted that k is expressed in the unit of min^{-1} here.



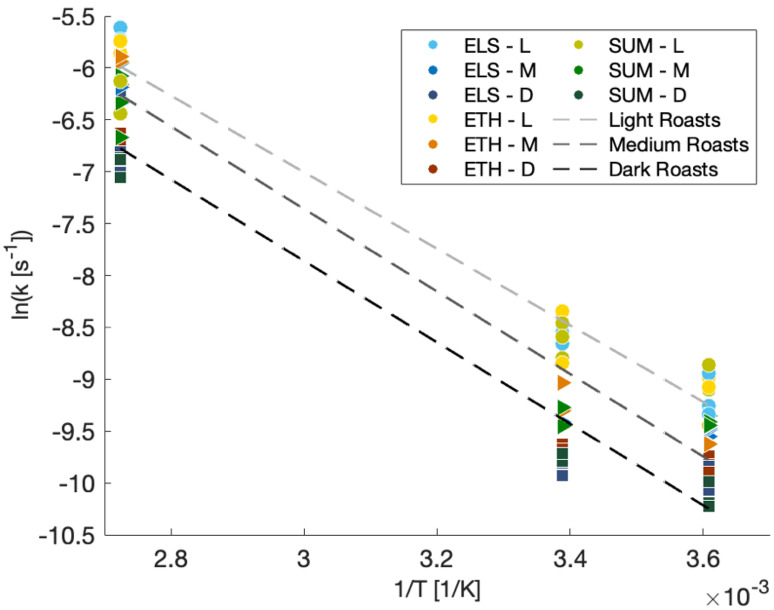
Supplementary Figure 3-S2C. Scatter plots of dynamic *TDS* over time of full immersion brewed coffee at $R_{brew} = 15$ of three origins at three roast levels brewed at 94°C (hot). Individual trial replicate regressions to the model equation $TDS = \left(C_{eq} - C_0\right)(1 - e^{-kt}) + C_0$ are indicated by lines; noted that k is expressed in the unit of min^{-1} here.



Supplementary Figure 3-S3. Scatter plots of Extraction yield over time of full immersion brewed coffee at **A)** 4°C, **B)** 22°C, **C&D)** 94°C three origins at three roast levels brewed under **A-C)** $R_{brew} = 5$ and **D)** $R_{brew} = 15$.



Supplementary Figure 3-S4. Boxplots of regressed values of individual trial replicates of full immersion brews at $R_{brew} = 15$ using coffee from 3 origins (ELS, ETH, SUM), 3 roast levels (L, M, D), and brewed at 94°C.yao



Supplementary Figure 3-S5. Arrhenius Plot of k and brewing temperatures of $R_{brew} = 5$ brews with best-fit lines at each roast level.

Coffee	Roast Level	Agtron Gourmet score (whole bean)
El Salvador Cerro Las Ranas Honey	Light	58.7 ± 1.4
	Medium	49.6 ± 1.2
	Dark	36.8 ± 1.5
Ethiopia Guji Washed organic	Light	57.0 ± 0.8
	Medium	49.5 ± 1.3
	Dark	36.8 ± 1.9
Sumatra Fair-Trade Organic Takengon	Light	56.1 ± 0.7
	Medium	49.2 ± 0.9
	Dark	38.1 ± 0.7

Supplementary Table 3-S1. Color score of roasted whole beans and coffee grounds measured in Agtron Gourmet scale.

Preparation Factors	C_{eq} (*TDS %*)	C_0 (*TDS %*)	k (hr^{-1})
Origin (processing)	3.58×10^{-7} *	0.939	0.0321 *
Roast	1.77×10^{-5} *	0.000593 *	1.96×10^{-7} *
Temperature	$< 2.2 \times 10^{-16}$ *	$< 2.2 \times 10^{-16}$ *	$< 2.2 \times 10^{-16}$ *
Origin : Roast	0.532	0.808	0.999
Origin : Temperature	0.248	0.568	0.0120 *
Roast : Temperature	0.00212 *	4.11×10^{-6} *	4.08×10^{-8} *

Supplementary Table 3-S2. P-values from the result of three-way Analysis of Variance with two-way interactions using Origin, Roast, and Brewing Temperature as factors and the fitting parameters (cf. Fig. 4) as response variables for all the $R_{brew} = 5$ brews. Established significance at 5% is indicated by asterisk.

Chapter 4. The effects of particle size and agitation on the extraction dynamics of full immersion brewed coffee

---

Author contributions:

Jiexin Liang co-designed the study, conducted experiments, performed data analysis and figure preparation, and wrote the original draft of the manuscript. Megan Dunkin and Hudson Brown conducted experiments and co-wrote the manuscript. William D. Ristenpart secured funding, co-designed the study, advised data analysis, revised and edited the manuscript.

In addition, the authors would like to acknowledge Joanne Yang and Karen G. at Peet's Coffee for conducting the particle grind size measurements.

4-1. Abstract

It is well established that the dynamics of coffee extraction depend on several brewing parameters, including temperature, grind size, brew ratio, and brew time. Another important but less-studied factor known to affect coffee extraction dynamics is agitation rate. Here we studied the effect of agitation rate on full immersion coffee brewed at 99°C using various types of agitation (continuous and interval) over a wide range of agitation speeds (rpm = 0 to 1200). We further examined how agitation rate affects extraction dynamics when the ground coffee particle sizes are varied over a wide range. We interpreted the extraction dynamics in terms of a model equation that includes an initial concentration (C_0), an equilibrium concentration (C_{eq}), and an effective mass transfer coefficient (k). Our experimental results indicate that k of the agitated brews, C_{eq} and the “rinse” ratio C_0/C_{eq} of all brews increased with decreasing particle size. However, at a constant grind size for the agitated brews, which k is independent of agitation rate suggesting that the extraction rate full immersion brewed coffee is limited by internal diffusion out of the coffee particulate even with increasing speeds of agitation. Moreover, even infrequent continuous and interval agitation (rpm =45) can speed up the extraction dynamics by more than a factor of two compared to non-agitated full immersion brews coffee. The practical implication of our finding is that grind size and agitation provides a useful tool for practitioners to fine-tune the extraction dynamics in full immersion coffee brewing.

4-2. Introduction

Coffee brewing is a complex process that involves the extraction of desirable compounds from coffee particle for a final cup of flavorful coffee beverages. As the simplest form of coffee brewing method, full immersion coffee was widely utilized because of its simplicity and robustness (Angeloni et al., 2019a; Gloess et al., 2013; Liang et al., 2021; Lingle and Menon, 2017). The brew strength and extraction yield are two important quantitative measurements of the extraction process of every coffee brew. Many factors contribute to the extraction of solubles and the corresponding physicochemical and sensory properties of the brew, such as the coffee origin, post-harvest processing method, roast level, and the brewing method, including important parameters like extraction time, mass/water brew ratio, temperature, grind size, and agitation rate. Prior studies have established that brew ratio primarily governs the final brew strength, while brewing temperature strongly affects the extraction rate and roast level weakly affects it, and the effect of origins or processing methods on the extraction dynamics are mostly negligible (Cordoba et al., 2020, 2019, Liang et al., 2023, 2021, n.d.; Rao et al., 2020; Voilley and Simatos, 1979).

In addition, the particle size of coffee grounds plays an important role in determining the extraction and sensory characteristics of the brewed coffee. Grinding roasted coffee beans facilitates the release of coffee aroma compounds from the grounds (Akiyama et al., 2003; Bhumiratana et al., 2011). Grinding further facilitates extraction of soluble materials by increasing the surface area to volume ratio. Coffee brewed with too fine of a grind can result in over extraction, concentrated taste, and heavy body, while too coarse of a grind can result in under extraction, lack of flavor, and a “watery” cup (Portela et al., 2022). Control over an optimal particle size is crucial by finding a balance between extraction efficiency and cup quality. Studies have shown that the extraction of soluble and aroma compounds varied inversely with particle size (Andueza et al., 2003a; Severini et al., 2015). For full immersion brewed coffee specifically, the effect of particle size on the extraction dynamics has also been well established. In un-agitated brews, the equilibrium *TDS* increases with smaller particle sizes, although this effect is relatively weak compared to the major effect of brew ratio for hot brews (Liang et al., 2021). Prior studies reported that the particle size does not significantly impact the equilibrium concentration of caffeine or 3-chlorogenic acids in cold brew (Fuller and Rao, 2017). Following a French press brewing method, Moroney et al. reported that finer grind size extracts faster and reach higher final concentration (Moroney et al., 2015). In agitated brews, it has been reported that the finer grinds resulted in higher concentration in the coffee brew (Voilley and Simatos, 1979; Wang and Lim, 2021). More precisely, Spiro et al. reported that the rate of extraction of caffeine varies inversely with the square of coffee particle radius (Spiro and Page, 1984; Spiro and Selwood, 1984).

Conversely, the effect of agitation rate was less studied, despite agitation being recognized as an important aspect of coffee brewing. Many full immersion methods involve some form of agitation. For example, French press includes a process of pressing down the brew to separate liquid and solid (Cordoba et al., 2020; Moroney et al., 2015), coffee cupping protocol requires "breaking the crust" (Lingle and Menon, 2017), and some cold brew methods involve stirring the mixture to ensure wetting of the grounds (Batali et al., 2022). Thus, there is a need to understand how agitation-related protocol effects the extraction of coffee. An early work in caffeine infusion indicated that the caffeine extraction rate is independent of the agitation speed

(Spiro and Page, 1984), while a more recent study reported that introduction of agitation to cold brew increases the extraction of solubles (Ahmed et al., 2019). No study to date has investigated the effect of agitation rate and agitation format on coffee extraction dynamics for a wide range of grind sizes, leaving unanswered how grind size and agitation interplay in governing the extraction dynamics of full immersion brewed coffee.

In our prior work, we adapted an diffusion-limited model for caffeine and proposed an updated and extended model for the extraction of all solubles using full immersion brewing technique (Liang et al., n.d.; Spiro and Selwood, 1984; Zanoni et al., 1992). This practical model was validated with wide range of brewing temperatures, roast levels, and coffee origins with different processing methods. That work did not examine, however, the impact of agitation rate or particle grind size.

Here, we study the effects of coffee grounds particle size, agitation rate, agitation format, and their interplay on the extraction dynamics of full immersion brewed coffee. We demonstrate that the extraction of solubles, as measured in total dissolved solids (*TDS*) using full immersion brewing technique, follows an internal diffusion-limited regime as evidenced by insensitivity to agitation rate above a small thrshold. Using the updated diffusion-limited model for full immersion brewed coffee, we further interpret the extraction dynamics results from a large experimental data set composed of coffee brewed at 99°C with 7 different grind size settings ranging from 360 to 1319 µm, and three different types of agitation with various agitation rate including no agitation, continuous agitation with a magnetic stirrer, and interval agitation with a spoon. The findings presented here provide valuable insight on how the control of particle size and introduction of agitation to full immersion brew can be utilized in achieving desired brew strength and extraction yield that aid in elevating the coffee cup quality.

4-3. Theory

Full immersion brew involves simply adding water to coffee grounds, so the brew ratio is defined by the mass of coffee grounds (M_g) and the mass of water (M_w),

$$R_{brew} = \frac{M_w}{M_g}. \tag{4-1}$$

Strength (TDS) and extraction yield (E) are two important quantitative measurements for every full immersion brew. TDS is the amount of solubles present in the liquid coffee beverage, while E is the fraction of solubles extracted from the coffee grounds during brewing. TDS can be easily measured experimentally using refractometry, and the instantaneous E can be calculated from TDS, since the two quantities are also related by the conservation of mass (Liang et al., 2021),

$$E = \frac{TDS}{1-TDS} R_{brew}. \tag{4-2}$$

In our previous work (Liang et al., n.d.), we adapted and streamlined an extant three-phase diffusion limited model for caffeine infusion (Spiro and Selwood, 1984; Zanoni et al., 1992), and proposed an "universal" full immersion coffee extraction equation (cf. Fig. 4-1B),

$$TDS = \left(C_{eq} - C_0\right)(1 - e^{-kt}) + C_0, \tag{4-3}$$

where C is the instantaneous concentration of the coffee solubles present in the liquid coffee brew (equivalent to the *TDS*), C_{eq} is the concentration of coffee solubles in both the wet coffee grounds and liquid coffee brew at equilibrium, C_0 is the initial concentration practically defined as the moment upon completion of water addition to the brew, and k is the effective mass transfer coefficient (Liang et al., n.d.).

The major assumptions of this model are that 1) we assume there is no accumulation at the solid/liquid interface of the individual coffee particulate, and that 2) the concentration of coffee solubles inside the wet coffee particulate rapidly reaches an effective equilibrium concentration, such that the mass transfer of coffee solubles is driven by the difference between the equilibrium concentration, which equals to the concentration of solubles inside the coffee ground, and the instantaneous concentration of coffee solubles in the external brew.

Previous work by Spiro et al. has established that diffusion of caffeine through the coffee bean particulate is the rate-limiting step, rather than the mass transfer across solid/liquid interface nor the diffusion through the Nernst layer in the bulk (Spiro and Page, 1984; Spiro and Selwood, 1984). For coffee particulates modeled as spherical particles with radius r, if the internal diffusion through particulate is the rate-limited step for all coffee solubles, then k can be expressed using the diffusion coefficient through the coffee particle, D_{bean}, of all extractable coffee solubles (Spiro and Selwood, 1984)

$$k = \frac{12D_{bean}}{r^2}, \tag{4-4}$$

in which k is inversely proportional to r^2. Contrariwise, if the diffusion through the Nernst layer is rate-determining, then k can be expressed using the diffusion coefficient in the solution, D_{soln}, of all extractable coffee solubles from the brew (Spiro and Selwood, 1984)

$$k = \frac{3KD_{soln}}{r\delta}, \tag{4-5}$$

where δ is the thickness of the Nernst layer around each particle, and K is the partition coefficient of all solubles between the coffee particulates and liquid brew, in which k depends on both r and δ. To compare the rate of internal diffusion versus external diffusion, one can vary r by varying the grind size of coffee grounds and vary δ by agitating the coffee brew.

Thus, this study focuses on assessing whether the internal diffusion rate-limited observations previously observed with just caffeine also pertains to all coffee solubles, by measuring the extraction rates over a wide range of agitation rates and particle grind sizes in full immersion coffee brews.

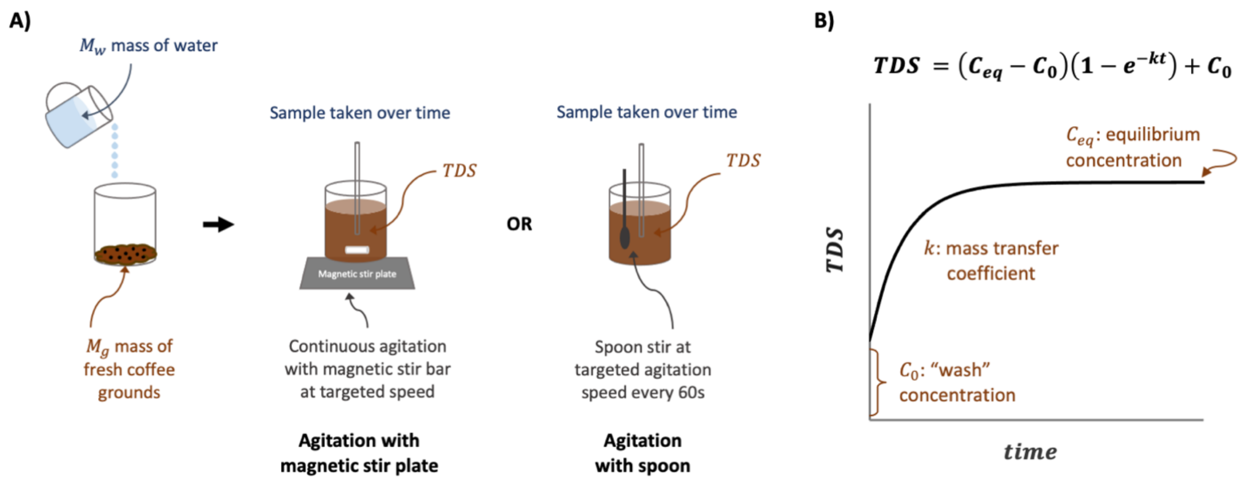


Figure 4-1. A) Definition sketch of full immersion brews with agitation on magnetic stir plate with stir bar or agitation using spoon. **B)** Illustration of universal full immersion brewing model equation Eq. (4-3) (Liang et al., n.d.).

4-4. Methodology

4-4.1 Coffee

A blend of washed processed African coffees composed of Rwanda Kivu Kanzu, Rwanda Kivu Kibuye, Rwanda Musasa Mbilima Dukunde, and Ethiopia Yirgacheffe Kebele Kochore was used in this study. Each coffee was roasted individually at the UC Davis Coffee Centre using a 1.5-kg Loring Demo Roaster (Loring Smart Roast, Inc., Santa Rosa, CA, USA) within a five-day period. The color of the roasted coffee were measured using an Agtron Analyzer with a score of 67.2, 70.0, 70.1 and 70.4, respectively on the Agtron Gourmet scale published by the SCA (Specialty Coffee Association, 2018). The coffee was allowed to de-gas for 2 days. Then, they were well mixed together, packaged in vacuum sealed plastic bags, and stored in a freezer at –20°C to ensure quality consistency (Cotter and Hopfer, 2018). The coffee was defrosted at room temperature one day prior to use.

4-4.2 General procedure for full-immersion agitated brews

For each trial, a constant brew ratio $R_{brew} = 15$ (600g water: 40g grounds) and a standard 1-L beaker was used. The coffee was first ground using a Mahlkönig Guatemala Lab Grinder (Mahlkönig USA, Durham, NC, USA) to a target grind size. Fresh coffee grounds were then measured out and added to the beaker. Water was heated to 99°C using an OXO Adjustable Temperature Pour-Over Kettle (OXO, New York City, NY, USA). Prior to starting the brew, the stir bar was added to the grounds and the beaker was placed onto a scale to measure the mass of water added. At the start of the trial, water was poured directly into the beaker in a circular motion to ensure even wetting of all the grounds. Samples were pipetted from the upper middle of the cone-shaped swirl formed by the stir plate, at a volume of 0.5-1 mL for each sample. Samples were taken at 15 second intervals for the first 90 seconds, at 1-minute intervals until 5 minutes, 7 minutes, 10 minutes, and then 5-minute intervals until 60 minutes. This sampling schedule was followed regardless of the agitation rate or format.

Each individual sample was centrifuged using a Thermo Fisher Scientific mySPIN 6 mini centrifuge (Thermo Fisher Scientific, Waltham, MA, USA) at 6000 RPM for approximately 5 minutes to separate the liquid brew from undissolved particles. A drop of the supernatant (approximately 0.25mL) of the centrifuged liquid sample at room temperature was pipetted into a digital refractometer (VST, Inc) to measure the *TDS*. The calibration of the *TDS* refractometer was conducted following the method specified in the "digital refractometer calibration" section of our prior study (Liang et al., 2021). Following this general procedure, additional brewing conditions, including variations in grind size, agitation rate, and agitation format, were implemented to examine extraction dynamics of agitated brews.

4-4.3 Agitation with grind size variation

The experiment was performed using grounds from 7 different grind sizes, each at 4 different agitation speeds: non-agitated, spoon-stirred at 45 rpm, and magnetic stirred at average speeds of 360 rpm and 658 rpm. The median particle size corresponding to settings 1 to 7 on a classic Mahlkönig grinder are 360 µm, 579 µm, 776 µm, 972 µm, 1160 µm, 1222 µm, and 1319 µm; the particle size distributions were measured using the sample method described in previous study (cf. Supplementary Figure 4-S1) (Liang et al., 2021). Each distinct brew was repeated in triplicate.

4-4.4 Agitation with magnetic stirrer (RPM)

The same coffee at grind size setting 5 with mean particle diameter of 1160.5 ± 28.8 µm were used in these trials. Two different stir plates (Fisherbrand™ RT Basic Magnetic Stirrers and Fisher Scientific Laboratory HotPlate / Magnetic Stirrer 11-500 from Thermo Fisher Scientific, Waltham, MA, USA), which covered a wider range of agitation rates, were used to study varied stir speeds. Full immersion brews were prepared using the method describe in section 3.2. Immediately after the water was poured, the beaker was transferred onto the magnetic stir plate and set to the desired RPM speed setting (cf. Fig. 4-1A). The coffee brews were conducted for a full hour on the magnetic stir plate. During the brew, the speed of agitation of the stir plate was measured by counting the rotations per minute (RPM) of the magnetic stir bar. To do so, a slow-motion recording of the stir bar (or stir plate magnet underneath the plate if the stir bar was not visible in the beaker) alongside a timer was taken. The number of rotations was manually counted from the video for a given time interval. The average RPM of these four settings were 380, 645, 844, and 1140. Each distinct brew was repeated for at least 4 replicates.

In addition, we also performed experiments where initially the brew was left unagitated, and then the agitation was suddenly activated midway through the brew. These combined “quiescent-then-agitated” experiments were conducted such that in the initial 30 minutes, the brew was left undisturbed, and then placed on the stir plate and stirred at an average speed of

347 rpm (lowest setting) for another 30 minutes. This process was repeated for 60 minutes quiescent, 20 minutes stirred at an average speed of 312 rpm.

4-4.5 Agitation with spoon

Since few coffee industry professionals have access to magnetic stir bars, we also examined the influence of stirring manually with a spoon (cf. Fig. 4-1A). These trials of spoon-agitating the coffee brews were conducted to investigate the effect of general stirring and understand how "breaking the crust" in coffee cupping might influence extraction. To stir the brew, the spoon was placed vertically in the beaker with the tip in bare contact with the bottom of the container. 3 rotations were made within 4 seconds, repeated once every minute throughout the brew. Similar brews were performed at the slower rates of 1 rotation per 4 seconds and 1 rotation per 10 seconds, each done once per minute. An additional set of trials was conducted with spoon stirring in a horizontal motion where the spoon was moved from one end of the beaker to the opposite end and back, repeated every minute. Finally, a "break the crust" method typically used for cupping was tested where the grounds at the surface of the beaker were pressed down with the spoon 4 minutes into the brew. All experiments were performed in triplicate.

4-4.6 Temperature controlled trials

All of the preceding brews were performed in beakers placed on a bench in room-temperature, without any external heating, to mimic conditions typically encountered in the coffee industry. As such, the brews naturally cooled down with time. To assess the impact of this temperature decrease, additional temperature control trials were performed using grind size setting 5 coffee and a K-type thermocouple secured to the lip of the beaker such that the probe was completely submerged in the brew. Data was logged continuously for 60 minutes with a sampling rate of 1 Hz, using an Omega HH806 thermocouple meter (Omega Engineering, Inc., Norwalk, CT, USA). The same procedure was followed as above using the same agitation rate setting and sampling time intervals as section 3.4. One trial was performed for each of the rotation speed settings. Then, an additional set of three temperature trials was performed in an insulated container with no agitation. During the experiments, the top of the beaker was covered with aluminum foil, which was removed to take samples at the aforementioned intervals.

4-4.7 Data Analysis

Data analysis were conducted using MATLAB R2020b (The MathWorks, Inc., Natick, MA, USA) and RStudio 2022.07.1 Build 554 (Posit, PBC, Boston, MA). All plots were generated using MATLAB R2020b. Non-linear regression of *TDS* data to brew time using Eq. (4-1) was conducted using the MATLAB built-in function *lsqcurvefit*, in which C_{eq}, C_0, and k served as the fitting parameters. Then, the corresponding best-fit parameters were evaluated MATLAB built-in function *nlparci* to return a 95% confidence interval. The adjusted R^2 value of the regression was calculated from MATLAB using the built-in function *fitnlm*, and the p-value was calculated using the MATLAB built-in function *coeftest*. Linear regressions of k over $1/r^2$ via Eq. (4-4) was performed using MATLAB built-in function *polyfit*. The correlation coefficient (R) and p-value of the data used for linear regressions were calculated using the MATLAB built-in function *corrcoef*, and the coefficient of determination R^2 of the regression was obtained using R built-in function *lm*. Analysis of Variance (ANOVA) for each of the fitting parameters was conducted at 5% significance level using the R built-in function *aov*, using Type III sums of squares (SS), where Agitation rate and Trial replicate were the factors. Parameter means determined to be significant for the experimental factors were then compared using Fisher's Least Significant Difference (LSD) using *LSD.test* in the "agricolae" package.

4-5. Results

4-5.1 TDS over time

The dynamic *TDS* over time data at various grind size and agitation are shown in Figure 4-2. Both agitated and non-agitated full immersion brews show a fast initial increase in *TDS* between $t = 0$ and $t = 5\ min$; the *TDS* increased much more gradually after this time, eventually reaching an apparent steady equilibrium *TDS* between $t = 20$ and $t = 30\ min$, depending on the exact conditions. The *TDS* increased steeply between $t = 0$ and $t = 5\ min$ for smaller grind sizes, while larger grind sizes approached equilibrium more gradually. Furthermore, the full immersion trials showed that the equilibrium *TDS* is dependent on the grind size. With all other conditions held constant, finer grind sizes reach higher equilibrium *TDS* than coarser grind sizes for both agitated and non-agitated brews. For example, coffee with grind size setting of 1 (360 µm) reached an average equilibrium *TDS* of $1.79 \pm 0.04\ \%$ after 30 min with no agitation and $1.85 \pm 0.12\ \%$ with stir plate agitation at 658 RPM, while a grind size setting of 7 (1319 µm) reached an average equilibrium *TDS* of $1.11 \pm 0.03\ \%$ with no agitation and $1.44 \pm 0.03\ \%$ with stir plate agitation at 658 RPM. The observed trends in *E* were similar to *TDS* (cf. Supplementary Figure 4-S2), such that finer grind sizes reached higher equilibrium values than coarser grind sizes and increased in *E* more sharply at the beginning of the brew. A grind size setting of 1 reached an average equilibrium *E* of 25.7% after 30 min with no agitation, and 27.4% at RPM = 658, while a grind size setting of 7 reached an average equilibrium *E* of 16.9% with no agitation, and 21.9% with stir plate agitation at RPM = 658.

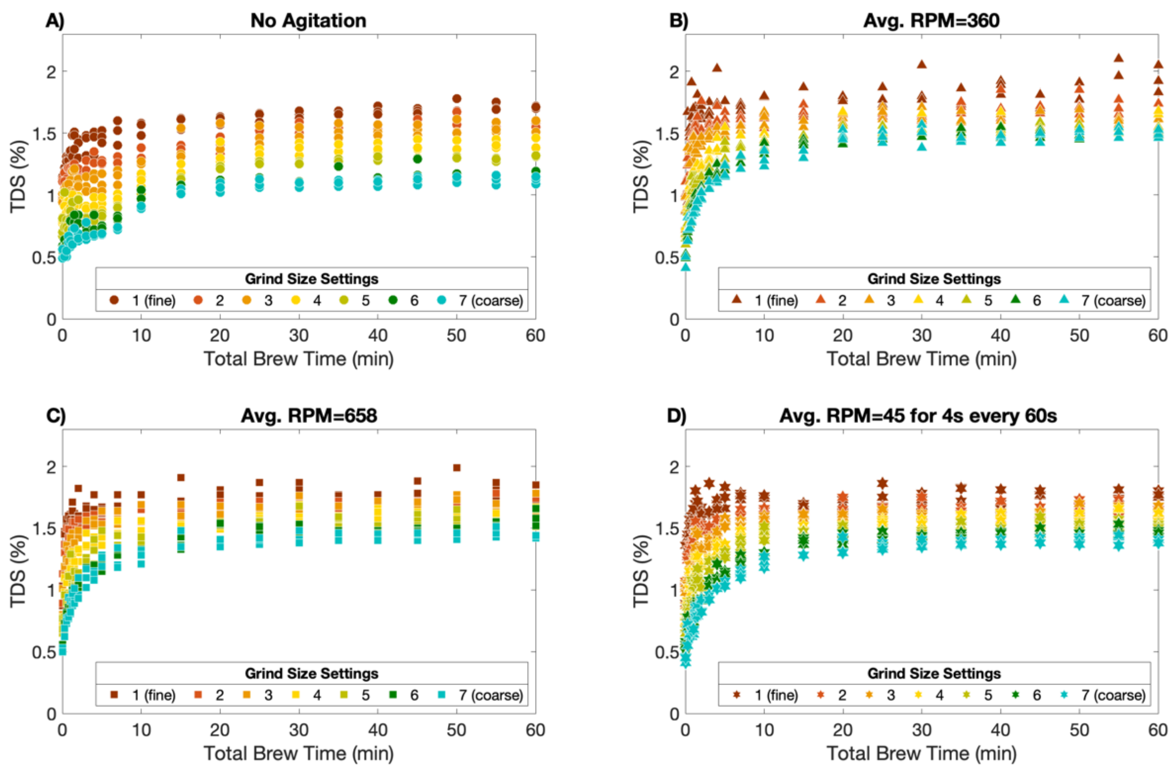


Figure 4-2. Scatter plots of the dynamic *TDS* of full immersion brews over time at various speed of agitation with different grind size settings corresponded to different particle sizes (cf. Table 4-1). The brews were agitated using a magnetic stir bar on a stir plate continuously at average specified speed, except the brews at rpm=45 were agitated with a spoon for 4 seconds every 60 seconds. Different agitation speeds are indicated by different shapes, and different grind size settings are indicated by different colors.

The agitated brews had more rapid increase in beginning of brewing and yield higher equilibrium *TDS* compared to the non-agitated brews. Overall, all three of the agitated trials displayed very similar trend of steep increase in the first ten minutes (cf. Figs 4-2B, C, D), and reached an average equilibrium *TDS* of 1.56 ± 0.11 %, which is around 10% higher than the non-agitated trials (cf. Fig 4-2A). In fact, interval agitation with a spoon also increased the *TDS* over time compared to the non-agitation brews. The spoon agitating trials also reached an average equilibrium *TDS* of 1.75 ± 0.06 % after 30 min for the finest grind size, and 1.39 ± 0.03 % for the coarsest grind size. Furthermore, additional trials with spoon stirring showed increase of *TDS* upon agitation is introduced into the brew process (cf. Supplementary Figure 4-S3). The "quiescent-then-agitated" trials reached similar equilibrium *TDS* values as the interval agitation with a spoon. "Breaking the crust" at the end of 4 min also resulted in an immediate increase of *TDS* upon agitation. However, these trials did not reach the same final *TDS* as the other constant agitated trials since "breaking the crust" is not continuous or interval agitation.

4-5.2 Comparisons of Extraction Dynamics at Various Grind Sizes

To characterize and compare the extraction dynamics of full immersion brew under various grind size and agitation, the experimental data from Figure 4-2 were fit to the "universal" full immersion coffee extraction model equation (Eq (4-3)) to obtain regressed values of C_{eq}, C_0, and k for each individual trial (cf. Figure 4-3). For all grind sizes tested, the agitated trials extracted faster than non-agitated trials, as indicated by higher values of k. Consistent with Fig. 4-2, the clearest trend is that varying grind size resulting in the change in surface area of coffee particles had a larger effect on k for agitated brews. Under a constant brew ratio, the effect of grind size on the extraction rate is much smaller in the quiescent brews than agitated brews. For example, in non-agitated brews, although there was variation at grind size setting 1, the coffee brews using grind sizes from setting 2 to 7 nonetheless exhibited an average k of $0.069 \pm 0.017\ min^{-1}$ without agitation. In comparison, the agitated brews also exhibited a larger range of k between $1.90 \pm 0.26\ min^{-1}$ for the finest grind size (setting 1) and $0.24 \pm 0.08\ min^{-1}$ for the coarsest grind size (setting 7), in which finer the grinds reached higher extraction rate, albeit with larger variations between trials. However, the impact of agitation is much smaller compared to the effect of grind size, as indicated by the observation that trials with different agitation rates are almost indistinguishable from each other.

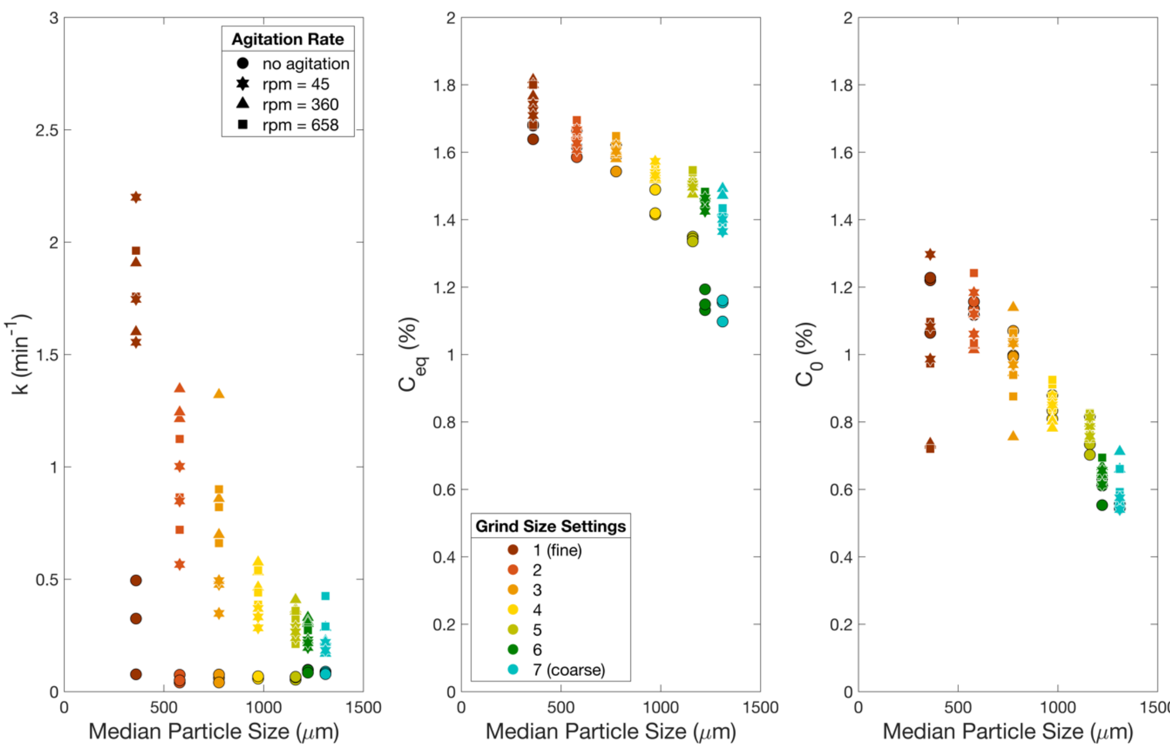


Figure 4-3. Scatter plots of regressed values of individual trial replicates of full immersion brews over particle sizes at various speeds of agitation. The regressed values equilibrium concentration (C_{eq}), initial concentration (C_0), and effective mass transfer coefficient (k) serve as the fitting parameters to the model Equation 4-1.

Similarly, the difference in C_{eq} and C_0 are also driven by grind size more than agitation rate, such that C_{eq} and C_0 increased with decreasing particle sizes, while the effect of agitation depended on grind size (cf. Figure 4-3B,C). The difference between agitated trials and non-agitated trials were pronounced in coarse grind sizes from setting 4 to 7. For the agitated trials, the finest grind size trials achieved an average C_{eq} of 1.75 ± 0.046 %, while the coarsest ones remained at 1.42 ± 0.044 %. Agitation had a larger effect on C_{eq} in coarse grind sizes, as the difference in C_{eq} between agitated trials and non-agitated trials increased with grind size. For example, the agitated brews at grind size setting 7 on average reached a 25% larger C_{eq} than the non-agitated brews. In contrast, the smallest grind size setting 1 yielded a C_{eq} only 5% larger when using agitation.

Similarly, brews with smaller particle sizes also reached higher initial concentrations, albeit with a larger scatter across trial replicates, especially with fine grind sizes. In fact, the "rinse" ratio, C_0/C_{eq} , which describes the rapid dissolution phase upon first contact with water, increased with smaller particle sizes (cf. Figure 4-4), although this trend becomes less clear with the grind size setting 1, due to a large scatter across trial replicates. The effect of agitation was likewise minimal on the "rinse" ratio, but the agitated trials with coarser grind sizes, settings 4 to 7, appeared to have lower "rinse" ratios than non-agitated trials, presumably due to higher values of C_{eq} with similar values of C_0.

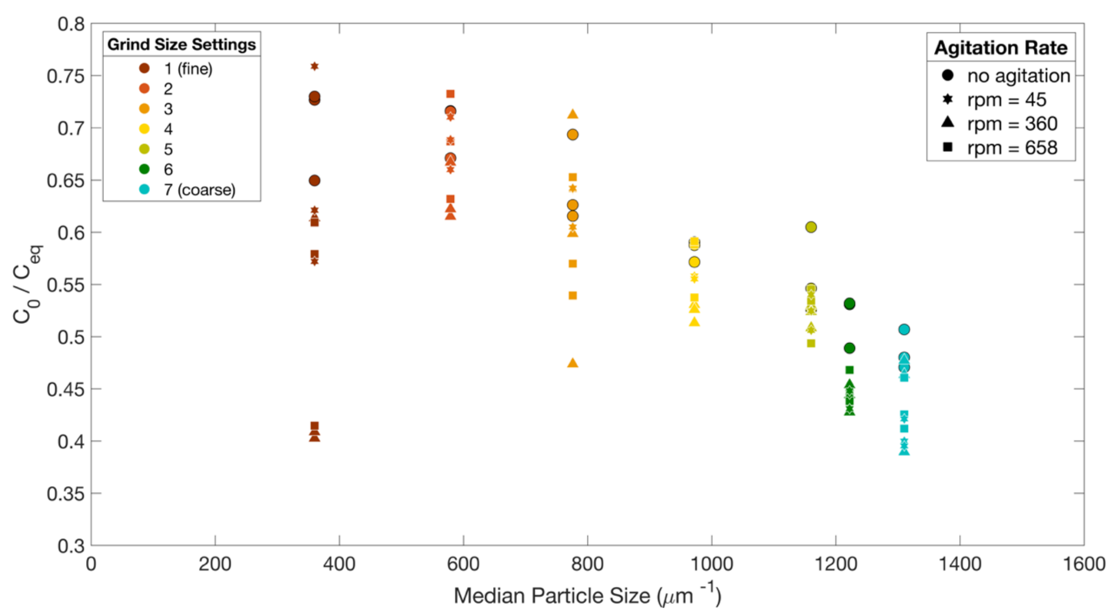


Figure 4-4. Scatter plot of the "rinse" ratio C_0/C_{eq} over particle size of individual trial replicates of full immersion brews over grind size settings at various speeds of agitation.

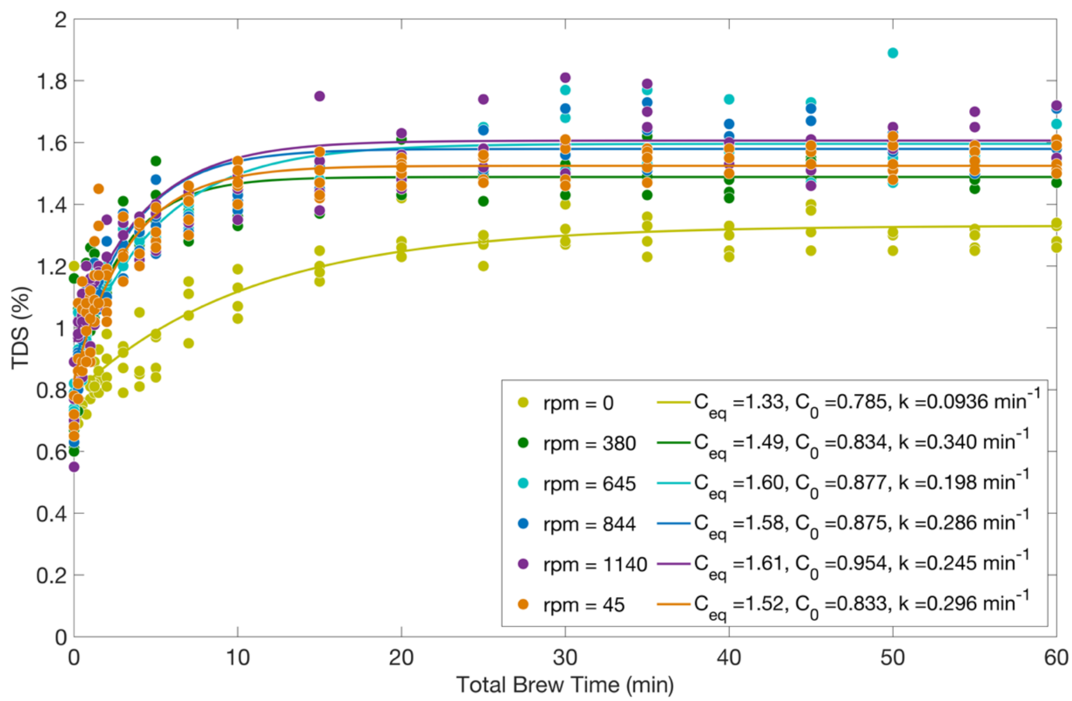


Figure 4-5. Scatter plot of the dynamic *TDS* of full immersion brews with grind size setting 5 over time at various speed of agitation. The brews were agitated using a magnetic stir bar on a stir plate continuously at average specified speed, except the brews at rpm=45 was agitated with a spoon for 4 seconds every 60 seconds. Regressions to the model Equation 4-1 across trial replicates are indicated by solid lines.

4-5.3 Effect of Agitation at Constant Grind Size

To further evaluate the effect of agitation on full immersion brews, the dynamic *TDS* a from trials with a larger range of agitation rates is shown in Figure 4-5. Under a constant grind size setting of 5, a sharp increase in both k and C_{eq} was observed between non-agitated and agitated brews. Coffee brews without agitation reached a C_{eq} of 1.33%, while the agitated brews reached an average C_{eq} of 1.56%; that is, full immersion brews with agitation reached 11-20% higher equilibrium *TDS* than non-agitated brews, with higher agitation rate reaching slightly higher equilibrium *TDS*. Furthermore, agitation dramatically increased the mass transfer rate of coffee solubles in full immersion brews. The quiescent coffee brews had a k of 0.0936 min^{-1}, while the agitated coffee brews reached an average k of 0.273 min^{-1}, nearly three times faster with agitation. The extraction rate of agitated coffee brews varied only weakly with agitation rate. Notably, trials with manual spoon-stirred agitation (RPM=45) had similar effects as the much faster magnetic stir plate constant agitation.

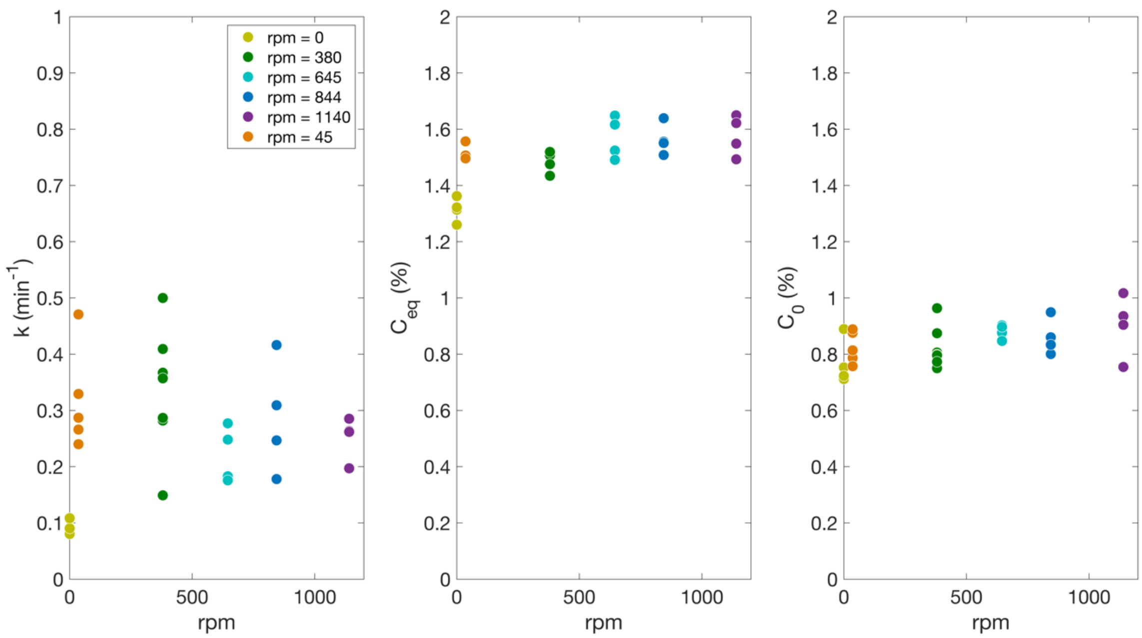


Figure 4-6. Scatter plots of regressed values of individual trial replicates of full immersion brews over various speeds of agitation with grind size setting 5 coffees. The dynamic *TDS* and *E* data are shown in Supplementary Figure 4-S2. The regressed values equilibrium concentration (C_{eq}), initial concentration (C_0), and effective mass transfer coefficient (k) serve as the fitting parameters to the model Equation 4-1.

The corresponding regressed values of C_{eq}, C_0, and k using Equation (4-3) from this set of agitation trials are plotted in Figure 4-6. The ANOVA results and parameter means are summarized in Supplementary Tables S1 and S2. Overall, the effect of agitation rate was significant on both C_{eq}, and k, while the impact on C_0 was not significant. The mass transfer coefficient k exhibited a threefold increase between no agitation to some agitation, as observed earlier. Further increases in agitation rate with the magnetic stir plate show large spread across trial replicates with an average of 0.29 ± 0.092 min^{-1}, yet the change in agitation rate for agitated brews had non-significant impact on k (cf. Supplementary Table 4-S2). The non-agitated trials had significantly lowered C_{eq} than all of the agitated trials, again with the spoon agitation yielding a similar effect on C_{eq} as the other constant agitation trials. For the magnetic stir plate constant agitation trials, C_{eq} significantly increased from RPM=380 to RPM=645, but C_{eq} did not increase further as the agitation becomes faster, even at a double agitation speed of RPM = 1145.

Supplementary Figure 4-S4 shows several more trials performed with additional agitation rates, including non-agitated trials with the thermally-insulated brewing condition. The trends are similar: introduction of agitation to full immersion brews increased the extraction rate and reached higher equilibrium *TDS* compared to no agitation, but the extraction dynamics were independent of agitation rate. Additionally, the insulated brew extracted faster than non-agitated trials, as expected because the brew remained hotter, but the higher temperature did not alter final equilibrium *TDS*.

4-5.4 The effective diffusion coefficient through coffee particle, $\boldsymbol{D_{bean}}$

Because the change in agitation rate within the range tested for the agitated brews did not have a significant impact on the extraction rate, the diffusion coefficient of coffee solubles through coffee particles can be estimated using linear regression of k over $\frac{1}{r^2}$ with all the agitated trials over various grind sizes (cf. Eq. (4-4)). Considering the agitated trials only, the external diffusion effect by varying agitation rate on extraction rates was not significant (cf.

Supplementary Table 4-2), while the internal diffusion was overall dominated as shown by the strong dependence of extraction rate on particle size especially in agitated trials (cf. Fig. 4-3). Additionally, a simple comparison of k over $\frac{1}{r^2}$ yielded a better fit than k over $\frac{1}{r}$ with a higher R^2 value (cf. Supplementary Fig. 4-S6). Linear regression over 63 agitated brewing trials yielded an average effective diffusion coefficient though the coffee particles of $D_{bean} = 9.37 \times 10^{-11}\ m^2/s$ for all coffee solubles in hot full immersion brews with initial water temperature at 99°C (cf. Fig. 4-7). Compared with previous studies, our prior study found that $D_{bean} = 4.08 \times 10^{-11}$ m^2/s at 94°C (Liang et al., n.d.), Spiro et al. reported $2.0 \times 10^{-10}\ m^2/s$ at 80°C for all coffee solubles (Spiro et al., 1989), and Zanoni et al. and Spiro reported values in the order of 10^{-11} to $10^{-12}\ m^2/s$ at 90°C (Spiro, 1993; Zanoni et al., 1992). Our D_{bean} estimation fall within the range of previous reported values, and presumably the discrepancy between our reporting values and the early reported values is due to differences in measurement methodology because these early studies measured the extraction yield using a oven drying method (Spiro, 1993; Spiro et al., 1989; Zanoni et al., 1992), which underestimates the true extraction yield (Liang et al., 2021). In addition, Zanoni et al. only measured the extraction rate from 1 min onward was used for their estimation (Zanoni et al., 1992). Furthermore, comparing with D_{bean} of caffeine, as one of the most studied coffee solubles, previous reported values are $1.73 \times 10^{-10}\ m^2/s$ at 84°C (Spiro and Selwood, 1984), and $3.2 \times 10^{-10}\ m^2/s$ at 90°C (Espinoza-Pérez et al., 2007). It is expected that D_{bean} for all solubles is smaller compared to caffeine's, because some coffee solubles are larger than caffeine, i.e. polysaccharides and melanoidins, resulting in an overall smaller effective diffusivity.

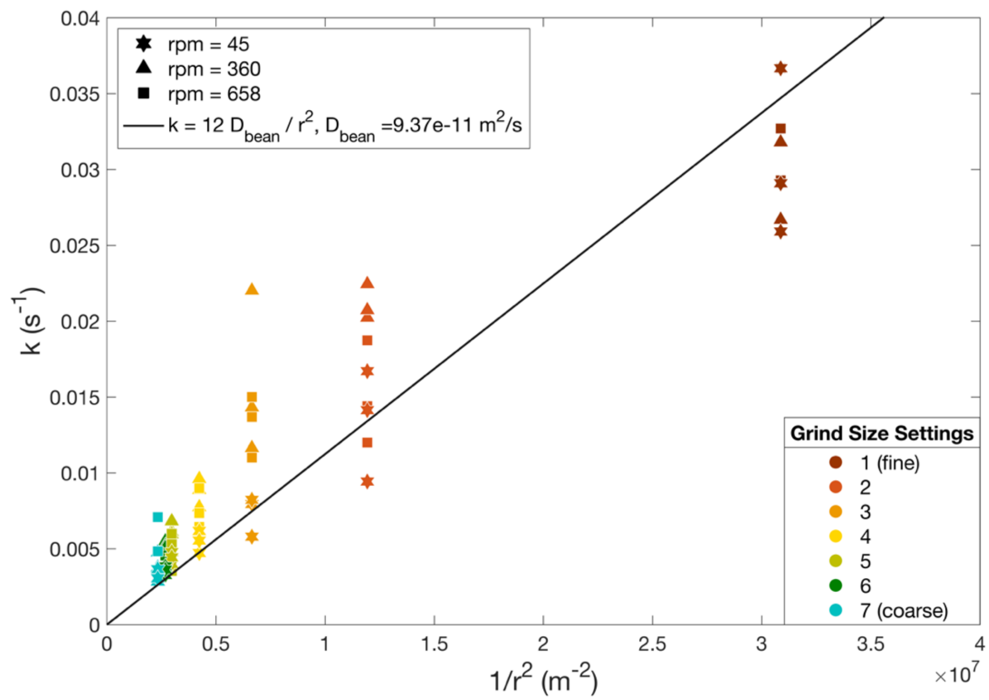


Figure 4-7. Scatter plot of the effective mass transfer coefficient k vs. $\frac{1}{r^2}$ for all the agitation brews with grind size variations. Solid black line is the linear regression with the data points to Equation 4-4 to estimation of diffusion coefficient through coffee particle, yielding $D_{bean} = 9.37 \times 10^{-11}\ m^2/s$.

4-6. Conclusion and Discussion

The overarching conclusion from this study is that the dynamic *TDS* profile, when tested over a wide range of grind size and agitation rate, invariably follows a diffusion-limited form of the "universal brewing curve" (Liang et al., n.d.). The important parameters C_{eq}, k, and C_0/C_{eq} all increase as the grind size becomes finer. Our results further demonstrated that the effective extraction rate of coffee solubles in full immersion brews is dominated by internal diffusion through the interior of the bean particles, in which k is independent of agitation rate.

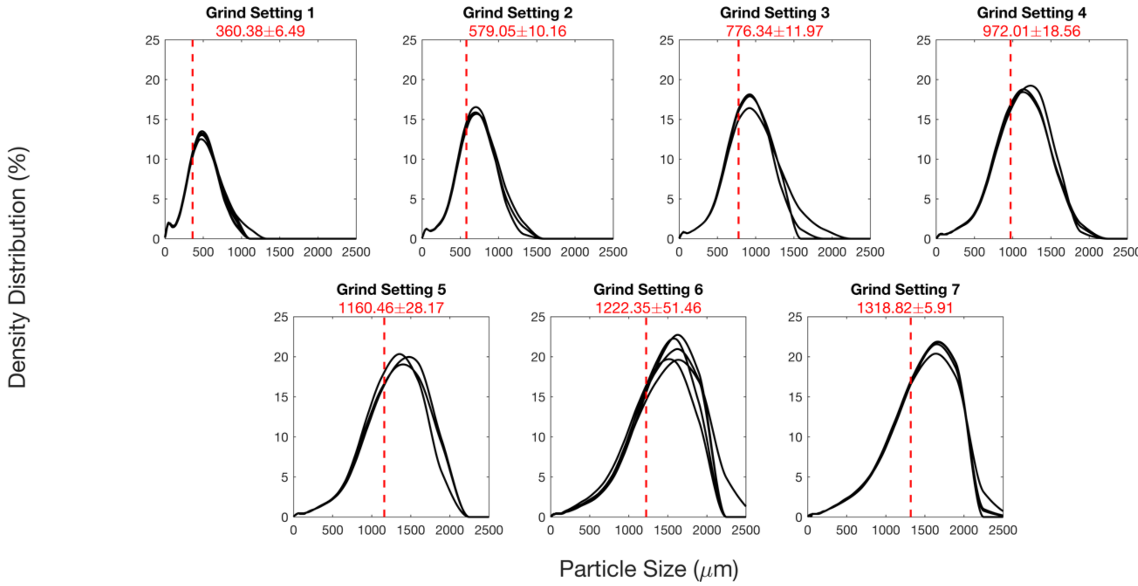
4-6.1 The diffusion-limited regime

It is unsurprising to find that the extraction kinetics was limited by the diffusion of coffee solubles through bean particle, as this finding has been established for caffeine extraction in full immersion coffee brews (Spiro and Page, 1984; Spiro and Selwood, 1984). While the diffusion coefficient depends on brewing temperature and degree of roast (Liang et al., n.d.; Spiro and Chong, 1997; Spiro and Hunter, 1985), several factors may contribute to the nature of low diffusion coefficient of coffee solubles through the coffee particles for similar reasons in caffeine diffusion (Spiro et al., 1989): (1) the counterflow of water into the coffee particles and gas releases simultaneously as coffee grounds are wetted (Maille et al., 2021); (2) porous nature of coffee particles results in tortuous diffusion path within the pores, hinders the movement of solubles (Welty et al., 2014); (3) the swelling of coffee particles further lengthens the diffusion path (Hargarten et al., 2020; Mo et al., 2022; Spiro et al., 1989); (4) slower diffusion caused by association between the species and insoluble components of the bean; and (5) association between soluble coffee species, such as the complex association between K^+ and caffeine, creating larger and slower-moving entities, further hindering diffusion through coffee particles (Jaganyi and Madlala, 2000).

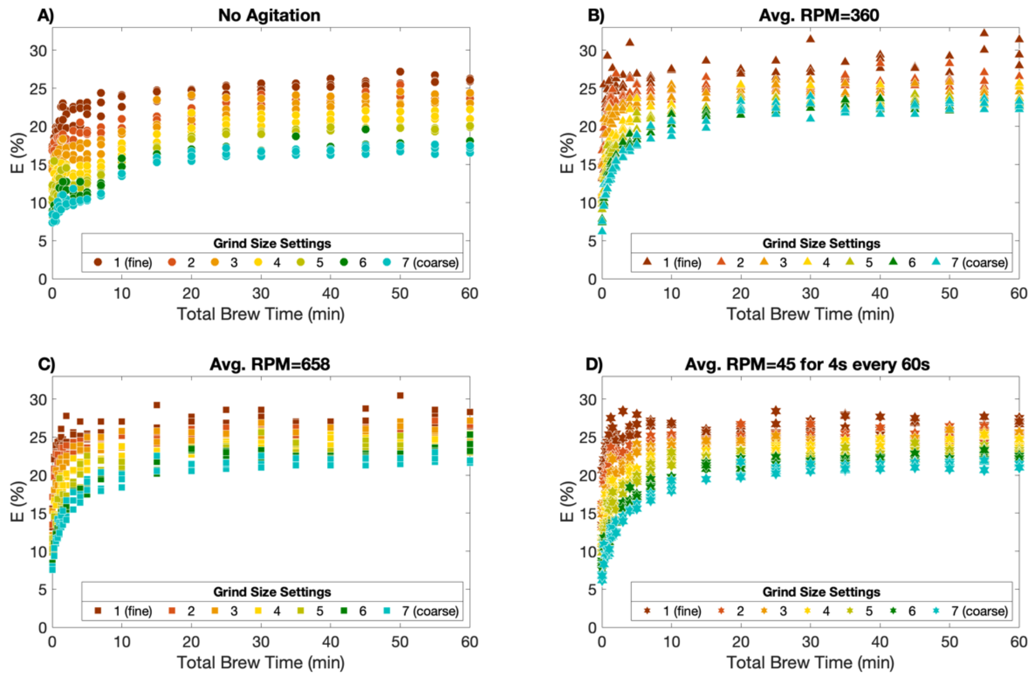
4-6.2 Practical implications

Full immersion brewing is simple and robust, because the equilibrium *TDS* can be coarsely adjusted via the brew ratio, while one has little control over the equilibrium *E* (Liang et al., 2021). Although the *TDS* is primarily determined by brew ratio, our results confirm that grind size provides a convenient tool to fine-tuning the brew to target specific *TDS* under a fixed brew ratio. For example, it allows one to move within a small region of *TDS* from 0.5% to 1.8% by changing grind size and brew time in quiescent brew (cf. Figure 4-2A). We emphasize, however, that coffee brewed with different grind size coffee grounds does not necessarily taste the same even with the control of brew time to yield identical strength, since coffee solubles and aroma compounds extraction also depend on extraction time (Lee et al., 1992; Mestdagh et al., 2014). Our work also confirms that a little bit of agitation goes a long way, in the sense that even intermittent slow agitation speeds up the extraction dynamics as much as continuous high velocity agitation. In other words, introduction of some non-zero amount of agitation immediately results in higher *TDS*, and constant agitation leads to increase in both extraction rate and equilibrium *TDS*, yet the extraction rate is independent of agitation rate. More specifically, under a constant brew ratio, grind size has a much smaller effect on the extraction rate in the quiescent brews, but grind size affects the extraction rate in agitated brews. Thus, coffee brewing partitioner should utilize grind size variations and agitation to gain control of extraction dynamics in achieving desirable strength and extraction in full immersion brews.

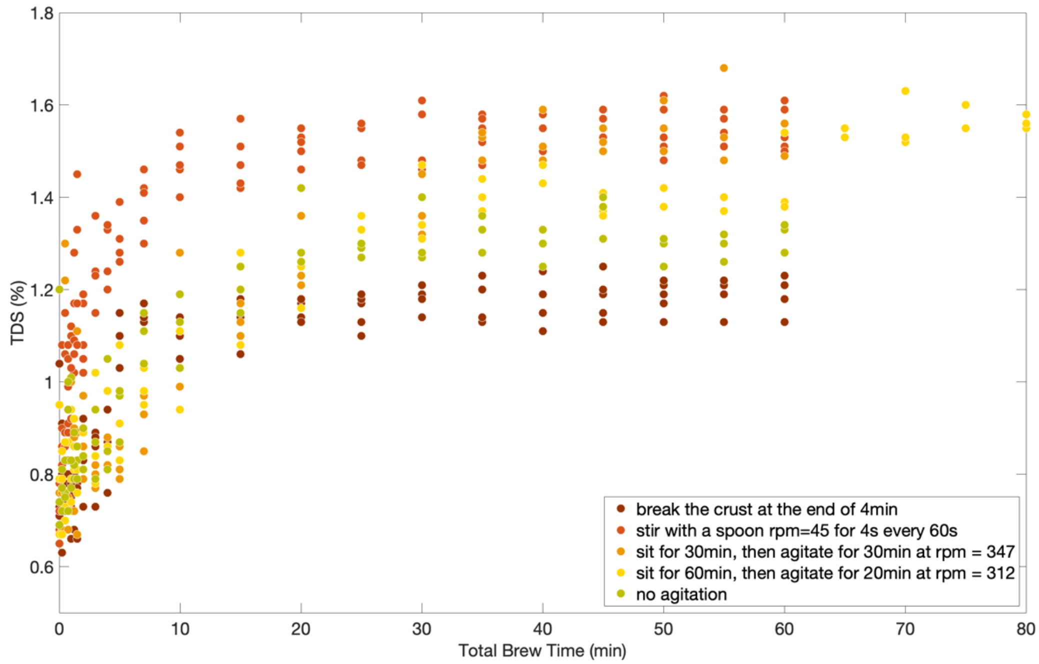
Supplementary Materials



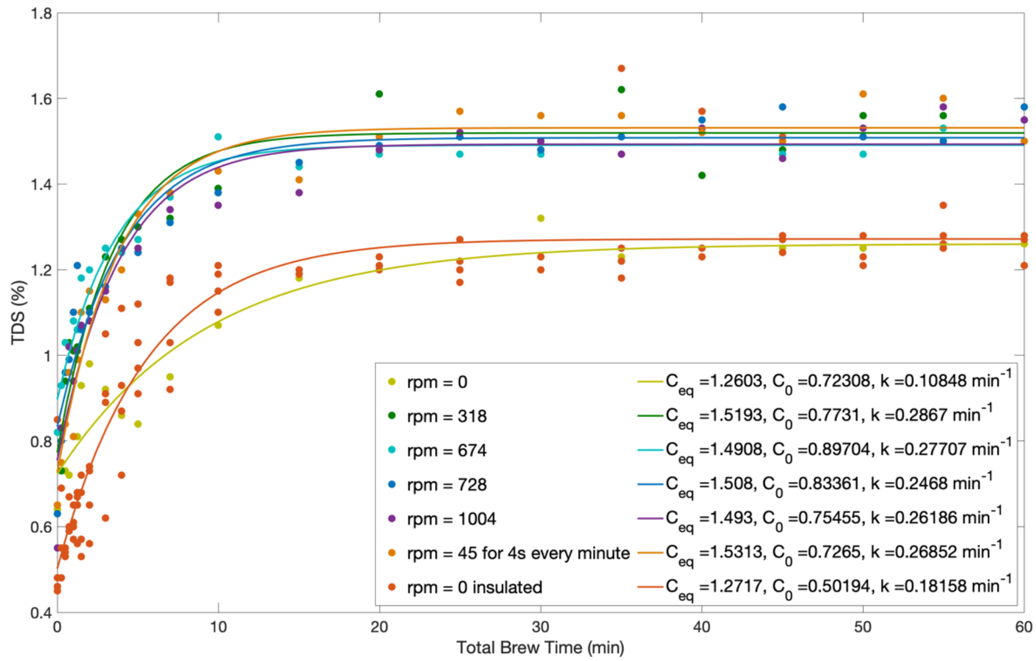
Supplementary Figure 4-S1. Particle size distribution at the seven grind size settings from the Mahlkönig Guatemala Lab Grinder. Distributions are expressed in the normalized differential density distributions of each given particle size. The median particle size with standard deviation at each grind size setting is indicated by red dashed line.



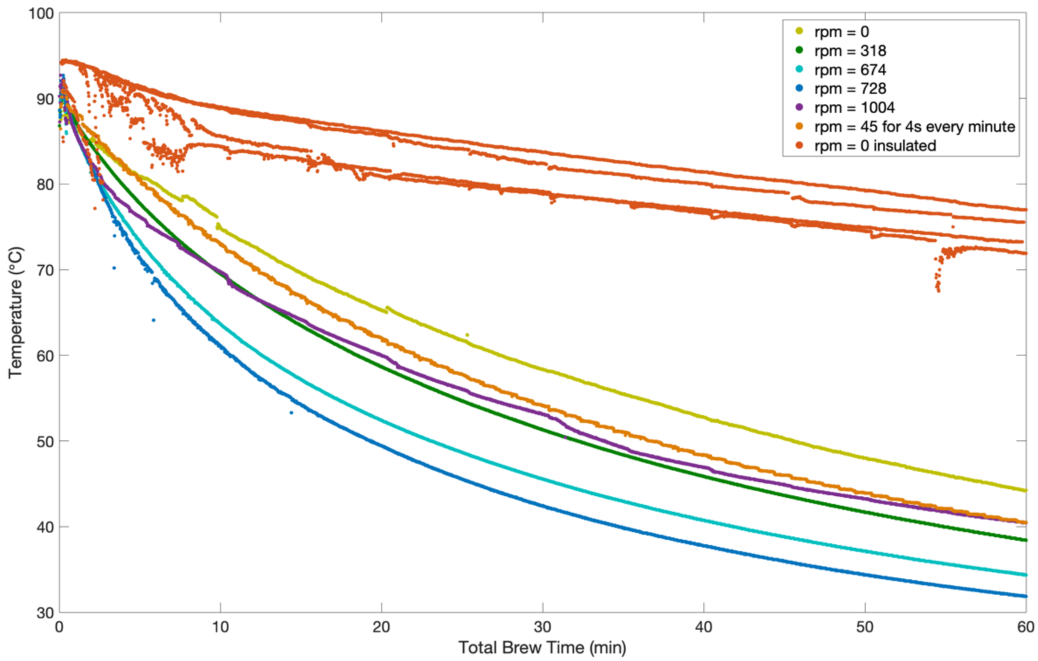
Supplementary Figure 4-S2. Scatter plots of the dynamic *E* of full immersion brews over time at various speed of agitation with different grind size settings corresponded to different particle sizes (cf. Table 4-1). The brews were agitated using a magnetic stir bar on a stir plate continuously at average specified speed, except the brews at rpm=45 were agitated with a spoon for 4 seconds every 60 seconds. Different agitation speeds are indicated by different shapes, and different grind size settings are indicated by different colors.



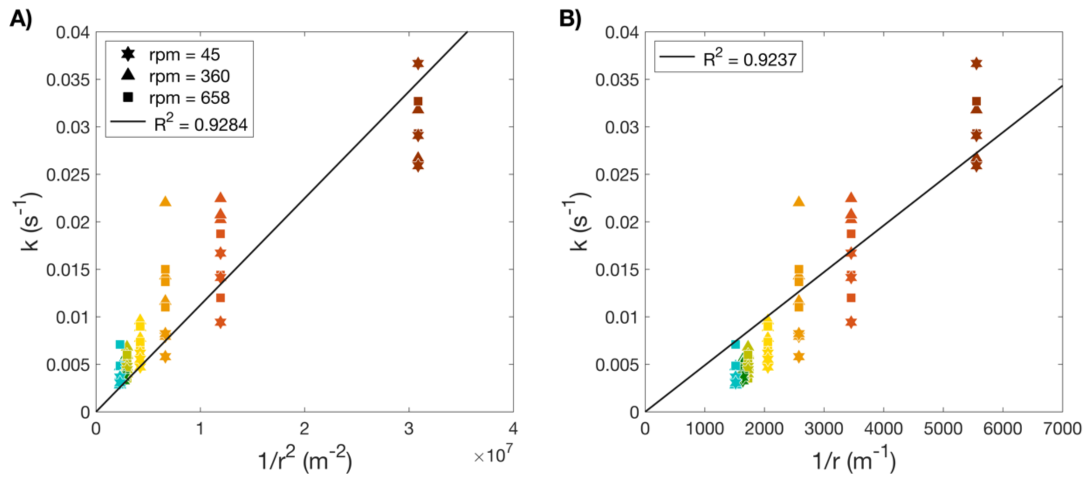
Supplementary Figure 4-S3. Scatter plot of the dynamic *TDS* of full immersion brews over time at different types of agitation.



Supplementary Figure 4-S4. Scatter plot of the dynamic *TDS* of full immersion brews with grind size setting 5 coffees over time at various speed of agitation. Different brewing conditions are indicated by different colors. Regressions to the model Equation 4-1 are indicated by solid lines. Note that, the insulated trials are colored in red, while all the other trials were un-insulated.



Supplementary Figure 4-S5. Scatter plot of temperature of full immersion brews (cf. Supplementary Figure 4-S4) at various agitation speeds over time.



Supplementary Figure 4-S6. Scatter plots of A) k vs. $\frac{1}{r^2}$ and B) for k vs. $\frac{1}{r}$ all the agitation brews with grind size variations. The linear fits through the origin with coefficient of determination R^2 are indicated in solid black lines.

Factors	k (min^{-1})	C_{eq} (*TDS %*)	C_0 (*TDS %*)
Agitation rate	0.0281 *	5.113×10^{-7} *	0.0866
Trial replicate	0.995	0.0313 *	0.0495 *

Supplementary Table 4-S1. P-values from the result of two-way Analysis of Variance using Agitation rate and Trial replicates as factors and the fitting parameters, k, C_{eq}, and C_0 (cf. Fig 4-6), as response variables. Established significance at 5% is indicated by asterisk.

Agitation Rates	k (min^{-1})	C_{eq} (*TDS %*)	C_0 (*TDS %*)
RPM=0	0.0965 [b]	1.314 [c]	0.769
RPM=380	0.336 [a]	1.497 [b]	0.823
RPM=645	0.221 [ab]	1.570 [a]	0.881
RPM=844	0.288 [a]	1.563 [a]	0.861
RPM=1140	0.252 [a]	1.578 [a]	0.903
RPM=45 (spoon)	0.319 [a]	1.523 [ab]	0.824

Supplementary Table 4-S2. Average regressed values of k, C_{eq}, and C_0 (cf. Fig 4-6) with Fisher's LSD significance codes for C_{eq} and k.

Chapter 5. Concentration Gradient Inversion via Sedimentation of Coffee Grounds in Full Immersion Brewing

Note: this chapter was based on published materials in *Journal of Food Engineering*

Jiexin Liang, Hudson G. Brown, Megan M. Dunkin, William D. Ristenpart, Concentration gradient inversion via sedimentation of coffee grounds in full immersion brewing, Journal of Food Engineering, Volume 357, 2023, 111619, ISSN 0260-8774, https://doi.org/10.1016/j.jfoodeng.2023.111619

Author contributions:

J.L. co-designed the study, conducted experiments, performed data analysis and figure preparation, and wrote the original draft of the manuscript. H.B. and M.D. conducted experiments, performed data analysis, and co-wrote the manuscript. W.D.R. secured funding, co-designed the study, advised data analysis, and co-wrote the manuscript. All authors revised and edited the final manuscript.

5-1. Abstract

In full immersion brewing methods, the coffee grounds are fully submerged in water during the brew and then filtered out prior to consumption. If the brew is not agitated, most of the coffee grounds quickly float to the surface, but then eventually sediment to the bottom as they de-gas and become less buoyant. Although this behavior is readily observed, little research has investigated the impact of the transient sedimentation process on the concentration profile of total dissolved solids (*TDS*) within the brew. Here, we report that unagitated full immersion brews undergo a concentration gradient inversion midway through the brewing process and that the time scale of the inversion depends sensitively on the roast level of the coffee grounds. Systematic measurements of the *TDS* versus both depth and time reveal that the brew contains a region of nearly twice the concentration near the top air/liquid interface at the beginning of the brew, but then the higher concentration region inverts to the bottom of the container as the brew progresses. Time-lapse photography observations indicate that the time scale of the gradient inversion is consistent with the average rate of sedimentation, which occurs up to a factor of three slower for darker roasts. A key implication of our results is that sensory evaluations obtained via the traditional "cupping" method used widely in the coffee industry might be confounded by differences in *TDS* for different roast levels.

5-2. Introduction

The general process of "full immersion" coffee brewing involves adding a specified quantity of hot water to a measured mass of coffee grounds placed in a container. Along with flow-based and pressurized brewing methods, full immersion brewing is one of the most commonly used coffee brewing techniques (Angeloni et al., 2019a; Cordoba et al., 2020). The most famous style of full immersion is arguably the French press, which despite its seeming simplicity engenders intense debates about the "best" way of using the press (Hoffmann, 2018; Wadsworth et al., 2021). More importantly, the full immersion brewing technique known as coffee "cupping" is widely used by coffee industry professionals around the world because of its simplicity and robustness (Lingle and Menon, 2017; Specialty Coffee Association, n.d.).

A key aspect of full immersion brews is that the individual coffee grounds are free to move around within the liquid. The initial pouring process mixes the liquid and grounds, but without further agitation some coffee grounds float upward and form a layer or "crust" on top of the liquid/air interface (Lingle and Menon, 2017). After the process of "blooming," during which gasses trapped in the grounds escape into the liquid and ambient air, the grounds gradually settle to the bottom of the brew (Hoffmann, 2018). The standard cupping procedure explicitly accounts for this transient behavior. After the hot water is poured on the coffee grounds most of the grounds float to the top immediately, and then after 3 to 5 min, the evaluator "breaks the crust" by stirring with a spoon (traditionally three times) to push down the coffee grounds while concurrently sniffing the coffee to evaluate the aroma. Skimming is performed shortly afterward to remove any remaining coffee grounds floating on the liquid surface. Then, in about 8 to 10 min, tasting evaluation of the liquid coffee begins.

The transient formation and dissipation of a floating crust is thus an integral part of widely used full immersion techniques, but prior scientific examinations of extraction in full immersion brews typically have used some form of agitation to eliminate the complex influence of sedimentation on the extraction process. For example, a typical laboratory method for measuring extraction rates is for the mixture of coffee grounds and water to be continuously stirred with a magnetic stir bar (Spiro et al., 1989; Spiro and Selwood, 1984; Zanoni et al., 1992; Spiro and Chong, 1997). Other agitation methods are also commonly used, including a stirring impeller (Voilley and Simatos, 1979), physically attaching coffee grounds to a rotating disc (Spiro and Page, 1984), or continuously shaking the mixture in the extraction process (Wang and Lim, 2021). Likewise, to measure the strength and extraction of full immersion brews, the standard approach is to filter the entire mixture through a filter paper to separate the spent grounds and liquid, then draw a sample from the liquid coffee to measure the total dissolved solids using a digital refractometer (Liang et al., 2021; Moroney et al., 2015). These approaches, however, focus on the extraction dynamics of the brew as homogenous mixture rather than as a non-homogenous mixture of the type that is typically sampled during the traditional cupping process. Specifically, to date there is no work that examines whether the transient sedimentation process affects concentration gradients within the brew due to the physical segmentation of liquid and solids.

Understanding how the transient sedimentation of the coffee grounds impacts the extraction process requires some consideration of the physics of sedimentation. In a quiescent liquid, an individual coffee ground particulate can be approximated as a sphere with radius a moving through a viscous liquid, such that a balance between gravity and viscous drag yields the Stokes sedimentation velocity,

$$v = \frac{2a^2\,\Delta\rho\,g}{9\mu}.$$

Here μ is the viscosity of the water, g is the gravitational acceleration, and $\Delta\rho$ is the density difference between the coffee ground and the water. A key complication for coffee is that $\Delta\rho$ changes dynamically with time. Coffee grounds are composed of a network of micro-scale pores that are initially filled with gas, meaning that $\Delta\rho < 0$ and the grounds move upward (i.e., they float to the top). As the gas escapes, eventually $\Delta\rho > 0$ and the coffee ground sinks.

Aside from the entrapped gas, one of the most important factors that affects the density of the coffee grounds is roast level. The walls of the porous network inside the coffee grounds are composed of a complex mixture of polysaccharides (Schenker et al., 2000). In coffee roasting, these polysaccharides undergo chemical degradation, and the porous cells themselves expand in volume because of the increasing internal pressure caused by water vapor and CO_2 formation (Redgwell et al., 2002). Due to the loosening cell wall structure as roasting proceeds, the bean density decreases, and porosity increases with roasting temperature (Bustos-Vanegas et al. 2018; Schenker et al. 2000; Ortolá et al. 1998). In general, the darker the roast, the lower the bean density. However, the bean density and porosity can also be affected by the roast profile. High-temperature short-time roasted coffee beans have lower density and higher porosity than low-temperature long-time roasted coffee (Schenker et al. 2000). Given the same particle size, the bulk density of coffee grounds decreases and bulk porosity increases from light to dark roast (Nakilcioğlu-Taş and Ötleş 2019; Ortolá et al. 1998). It remains unclear how the density and porosity resulting from a particular roast level will impact the dynamics of extraction in a full immersion brew.

The main goal of this paper is to elucidate the rate of sedimentation of coffee grounds and to characterize the corresponding concentration gradient of the total dissolved solids (*TDS*) present in full immersion brews over time, for three different roast levels (light, medium, dark). We demonstrate that an inversion in the concentration gradient occurs midway through the brewing process: initially the *TDS* is twice as high near the top surface, but the high *TDS* region inverts to the bottom as the coffee grounds sediment. We further demonstrate that darker roast coffee both sediments and extracts more slowly compared to lighter roasts, a finding we attribute to the lower density of the dark roast. Finally, we discuss the implications for the coffee industry, since our data suggests the sampling position of non-homogenized full immersion coffee brews can introduce large confounding variations in strength and sensory measurements.

5-3. Methodology

5-3.1 Coffee

An Arabica honey-processed coffee from El Salvador Cerro Las Ranas was used in this study. The coffee was roasted on a single day to three different roast levels (Light, Medium, and Dark) at the UC Davis Coffee Center using a Probat P-5 drum roaster (Probat-Werkevon Gimborn Maschinenfabrik GmbH, Emmerich am Rhein, Germany). The roast profiles of different roast levels are shown in Supplementary Figure 5-1. The colors of roast levels for whole beans were 58.7 for light roast, 49.6 for medium roast, and 36.8 for dark roast (Table 5-1), gauged by the Agtron Gourmet Color Scale published by the SCA (Specialty Coffee Association, 2018). The coffee was allowed to rest in bins at room temperature for a week after roasting to allow for de-gassing, and then vacuum-sealed in bags, and stored in a −20 °C freezer as a means of maintaining sensory quality consistent with previously published coffee sensory studies (Batali et al., 2022, 2020b; Cotter and Hopfer, 2018; Cotter et al., 2021). Each individual bag of coffee was defrosted overnight to room temperature before use.

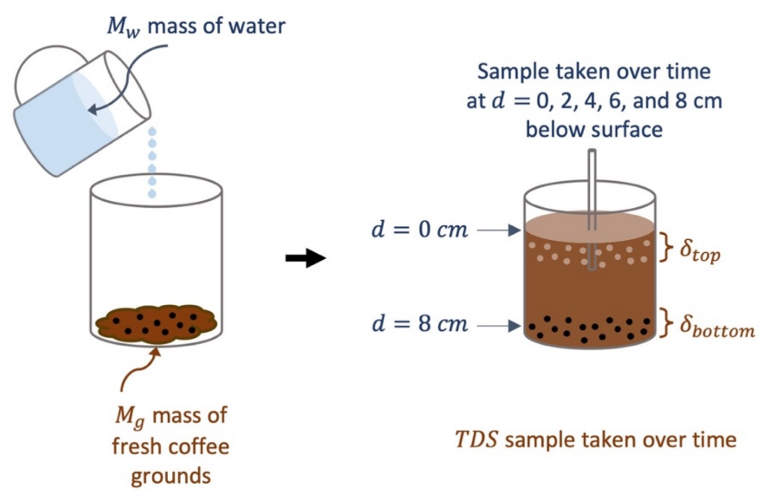


Figure 5-1. Schematic of the full immersion brew experimental procedure.

A schematic illustration of the experimental brewing procedure is shown in Figure 5-1. Three trial replicates were performed at each roast level (light, medium, and dark), yielding 9 total brews for the extraction measurements. The roasted coffee beans were ground to a median particle size of 1160.5 ± 28.8 µm at grind size setting 5 on a Mahlkönig Guatemala Lab Grinder (Mahlkönig USA, Durham, NC, USA). A brew ratio $R_{brew} = 15$ was used (600 g water to 40 g coffee grounds) for all spatiotemporal extraction dynamics trials. To visualize the coffee grounds during the sedimentation process, transparent 1 L glass beakers with height of 15.4 cm and diameter of 10.8 cm were used for all brews. For each brew, 40 g of coffee grounds of a particular roast level were placed into an empty beaker. After adding the coffee grounds, water heated to 99°C was poured into the beaker using a Bonavita 1.0-L Variable Temperature Electric Kettle (Bonavita World, Woodinville, WA). A circular pouring motion was used to ensure all grounds were fully wetted during the pouring process. The initial water temperature was 99°C, but to mimic typical brewing conditions we did not provide any heating to maintain the temperature and let it cool naturally. The ambient temperature was in the range of 21 to 24°C for al experiments.

Physical Measurements	**Roast Levels**		
	Light	**Medium**	**Dark**
Agtron Score of Whole Beans	58.7 ± 1.4	49.6 ± 1.2	36.8 ± 1.5
Bulk Density (g/mL)	0.35 ± 0.021	0.32 ± 0.002	0.30 ± 0.004
Tapped Bulk Density (g/mL)	0.42 ± 0.013	0.37 ± 0.005	0.34 ± 0.006

Table 5-1. Agtron scores of roasted whole coffee beans, and average bulk densities of loose and tapped coffee grounds at light, medium, and dark roast levels. All measurements represent the average plus or minus one standard deviation of triplicate measurements (N=3).

5-3.2 Spatiotemporal Extraction Dynamics

Immediately after completion of the pouring process, we began acquiring small samples (approximately 0.5 mL per sample) with a pipette to measure the *TDS* versus both time and position inside the beaker. Individual samples were obtained at every minute from 0 to 5 min, at 7 min, at 10 min, and every 5 min thereafter until 60 min had transpired (18 total time points). At each time point, we sequentially acquired an individual sample at five different depths measured from the top surface: d = 0, 2, 4, 6, or 8 cm. Thus, from each brew replicate we obtained a total of 90 samples versus time and depth. All sampling was performed as close to the radial center of the beaker as possible; preliminary measurements indicated negligible differences in the *TDS* sampled at the same depth but different radial positions.

Each sample was immediately centrifuged using a Thermo Fisher Scientific mySPIN 6 mini centrifuge at 6000 RPM (Thermo Fisher Scientific, Waltham, MA, USA) for 5 min to separate liquid brew from undissolved particles, and then allowed to cool down to room temperature. A drop of the supernatant (approximately 0.25mL) of the centrifuged liquid sample was then placed in a digital refractometer (VST, Inc) to measure the *TDS*. Calibration of the *TDS* meter was conducted following the same procedure specified in the "Digital refractometer calibration" section of a previous study (Liang et al., 2021).

5-3.3 Sedimentation Image Capture and Analysis

5-3.3.1 Image Capture

We also performed several separate brews to characterize the sedimentation behavior using time-lapse photography. In addition to the brews with 40g of coffee grounds investigated in spatiotemporal extraction dynamics as discussed above, we also investigated a larger volume coffee brew at the same brew ratio to compare the effect of batch size on coffee grounds sedimentation. Three trial replicates for each roast level (light, medium, and dark) at two different masses of grounds (40 g and 60 g) at a fixed brew ratio, $R_{brew} = 15$, were performed (600 and 900 grams of water, respectively), for a total of 18 sets of time-lapsed images. We pipetted out small samples from the brew following the same sampling schedule and method described in section 2.2 to make sure that the minor physical agitation introduced to the brew was consistent with the spatiotemporal extraction dynamics experiments. The time-lapsed photos were taken using a Nikon D5300 digital camera (Tokyo, Japan) at 1/30 shutter speed, 5.6 focus, and 125 ISO inside of a lightbox. The camera was programmed to take one image every 2 s for 32 min, resulting in a total of 960 images per trial. The time-lapse photography began concurrently with the pouring.

5-3.3.2 Image Analysis

The sedimentation time lapses were analyzed using the image analysis software package ImageJ (Schneider et al., 2012). Because the brews were opaque, the sedimentation behavior of individual coffee grounds was difficult to characterize. We instead focused on quantifying the overall thickness of the crust at the top (δ_{top}) and the sedimented layer at the bottom (δ_{bottom}), both of which changed with time.

The first image in each trial to be analyzed was the one immediately after completion of the pouring process where the chaotic mixing flows had appreciably ceased, which typically occurred within 10 s to 15 s after pouring; this image was identified as $t = 0$. Starting from this image, every other image was analyzed using the “multi-point” function in ImageJ, in which the top and bottom coordinates for each of the top and bottom layers of grounds were identified. In this manner, the thickness δ of each layer versus time was obtained (cf. Fig. 5-1). Two data points representing the height of the beaker were also taken, and this measurement along with the actual measured height of the beaker was used to calculate the conversion factor between pixels and centimeters.

For the 40-g brews, the four data points indicating the thicknesses (δ) of the top layer (δ_{top}) and bottom layer (δ_{bottom}) were taken consistently in the center of the beaker for all trials. Images every 4 s were analyzed throughout the 30 min. For the 60-g brews, during periods of very rapid sedimentation, every image was analyzed. Often a few individual coffee grounds became enmeshed in the bubbles at the surface of the brew, but we discounted these lone particles and defined the crust thickness as the distance over which the solid coffee particulates formed a clearly contiguous layer. Thus, any regions with majority foam or bubbles present at the surface of the brew without obvious presence of coffee grounds were not included as part of the top layer measurement. (A specific example of distinction between foam or bubbles and coffee grounds layer is illustrated at $t = 0\ min$ for medium roast in Supplementary Fig. 5-S2) In the 40-g brews, the thickness measurements were consistently taken from the center of the beaker. In the 60-g brews, in some trials the apparent thickness varied with position (i.e., it was thicker in some places than others); in these cases, we measured the thickest section of grounds. The image sets were analyzed fully or until no more appreciable sedimentation occurred, such that the thickness of the top layer was effectively zero.

5-3.4 Bulk Density Measurements

The bulk densities of both the loose and tapped coffee grounds at light, medium and dark roast levels were measured using standard methodologies (Amidon et al., 2017; Mitterlehner et al., 2021). For the measurement of loose coffee grounds bulk density, 15 g of coffee grounds were placed into a 100 mL graduated cylinder without compacting, and the volume of coffee grounds was measured and recorded. For the tapped bulk density, the procedure was the same except the graduated cylinder was tapped on a hard surface until the volume of the sample remained constant. The corresponding bulk density and tapped bulk density was calculated based on the mass of coffee grounds divided by the volume of loose or tapped coffee grounds, respectively. All measurements were performed in triplicate. The resulting tapped densities ranged from 0.42 g/mL for light roast to 0.34 g/mL for dark roast, i.e., the light roast was 24% more dense than the dark roast (Table 5-1).

5-3.5 Data and Statistical Analyses

The experimental data was compiled and analyzed in MATLAB R2020b (The MathWorks, Inc., Natick, MA). Two key metrics were: (1) the *TDS* inversion time $t_{TDS,in}$, defined as the time at which the *TDS* sampled at the surface (0 cm) became smaller than the *TDS* sampled at the bottom of brew (8 cm); and (2) the coffee bed thickness inversion time $t_{bed,in}$, defined as the time at which the thickness of the bottom bed first exceeded the thickness of the top bed. We also calculated the "sedimentation percentage," characterizing the fraction of grounds that had sunk to the bottom, defined as

$$sedimentation\ ratio = \frac{\delta_{bottom}}{\delta_{top}+\delta_{bottom}} \times 100\% \quad (5\text{-}1)$$

Running averages of the grounds thickness (cf. Fig. 5-3 and Supplementary Fig. 5-S3), as quantified via the digital image analysis (cf. 2.3.2) were calculated using the MATLAB built-in function *smooth* with a moving average span of 50 consecutive data points. The correlation coefficient (R) and p-value of the corresponding linear regressions were calculated using the MATLAB built-in function *corrcoef*. The uncertainties of $t_{TDS,in}$ and $t_{bed,in}$ were calculated by the standard deviation between trial replicates, except the uncertainties of $t_{TDS,in}$ of dark roast is calculated by measurement error. All plots were generated using MATLAB R2020b (The MathWorks, Inc., Natick, MA).

5-4. Results

5-4.1 Sedimentation Observations

As anticipated, transient floating then sedimentation of the coffee grounds was observed in all coffee brews. Representative images of the dynamics for light, medium, and dark roasted coffee are shown in Figure 5-2 (top, middle, and bottom rows, respectively; see also Supplementary Videos 5-S1, 5-S2, and 5-S3). The general process of sedimentation started with the majority of coffee grounds rapidly floating to the top air/liquid surface, then with individual particles slowly sedimenting to the bottom as brewing proceeded, culminating with the majority at the bottom by the end of a 30-min brew. At $t = 0$ min, the top layer of coffee grounds containing foam was invariably much thicker than the bottom layer across all roast levels in a given brew, indicating that almost all the grounds floated upward to the surface immediately after the addition of water. After that, the thickness of the top layer gradually decreased and the thickness of bottom layer increased with time (cf. series of vertical arrows in Fig. 5-2).

Importantly, the time-lapse images reveal that the dynamics differ appreciably for the different roast levels. The thickness of the layers for the light and medium roast changed much more rapidly than for the dark roast (cf. Figs. 5-2 and 5-3). In these representative trials, the top layer near $t = 2$ min was approximately 2 cm regardless of roast level, but by $t = 10$ min, for example, the top layer of the dark roast had hardly changed about 1 cm, while the top layer of the light and medium roasts had shrunk by more than 1 cm. At all times the thickness of top layer in dark roast was much thicker compared to the other two roast levels, with an average top layer thickness over time of $0.56 \pm 0.46\ cm$ for light roast, $0.97 \pm 0.58\ cm$ for median roast, and $1.42 \pm 0.41\ cm$ for dark roast. In other words, the light and medium roast coffee grounds sank much more quickly than the dark roast. Similar qualitative trends were also observed with the larger 60-g brews (Supplementary Figs. 5-S2 and 5-S3).

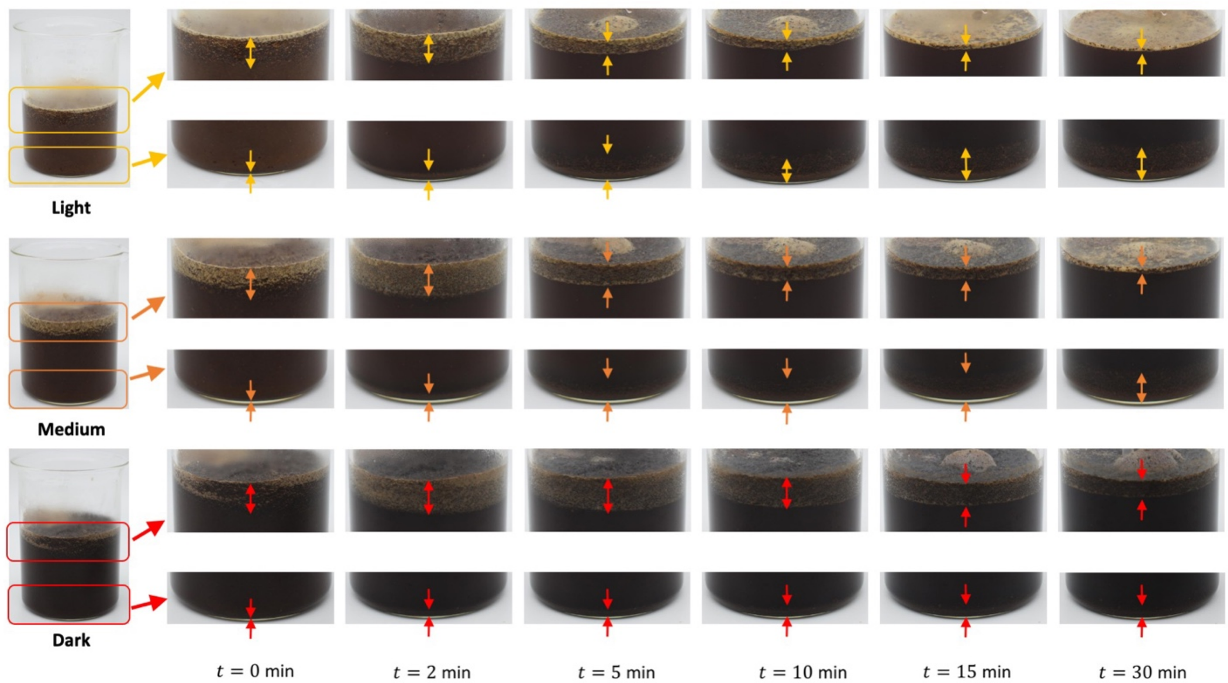


Figure 5-2. Representative images of full immersion 40-g brews and with light, medium, and dark roast coffee at 0, 2, 5, 10, 15, and 30 min of brew time. The thickness of coffee ground beds at the top and bottom are indicated by arrows. See also supplementary videos 5-S1 through 5-S3.

Our quantitative image analysis provided insight on the precise dynamics of the sedimentation process. The thickness of the coffee ground layers for the 40-g full immersion brews with light, medium, and dark coffee are shown in Figure 5-3. Consistently across all roast levels, the thickness of the coffee ground layer on top started almost immediately at 2-cm thickness, then decreased over time. Concurrently, the thickness of the bottom layer started near zero and increased with time to 1 cm for light and medium roasts, and to 2 cm for dark roast.

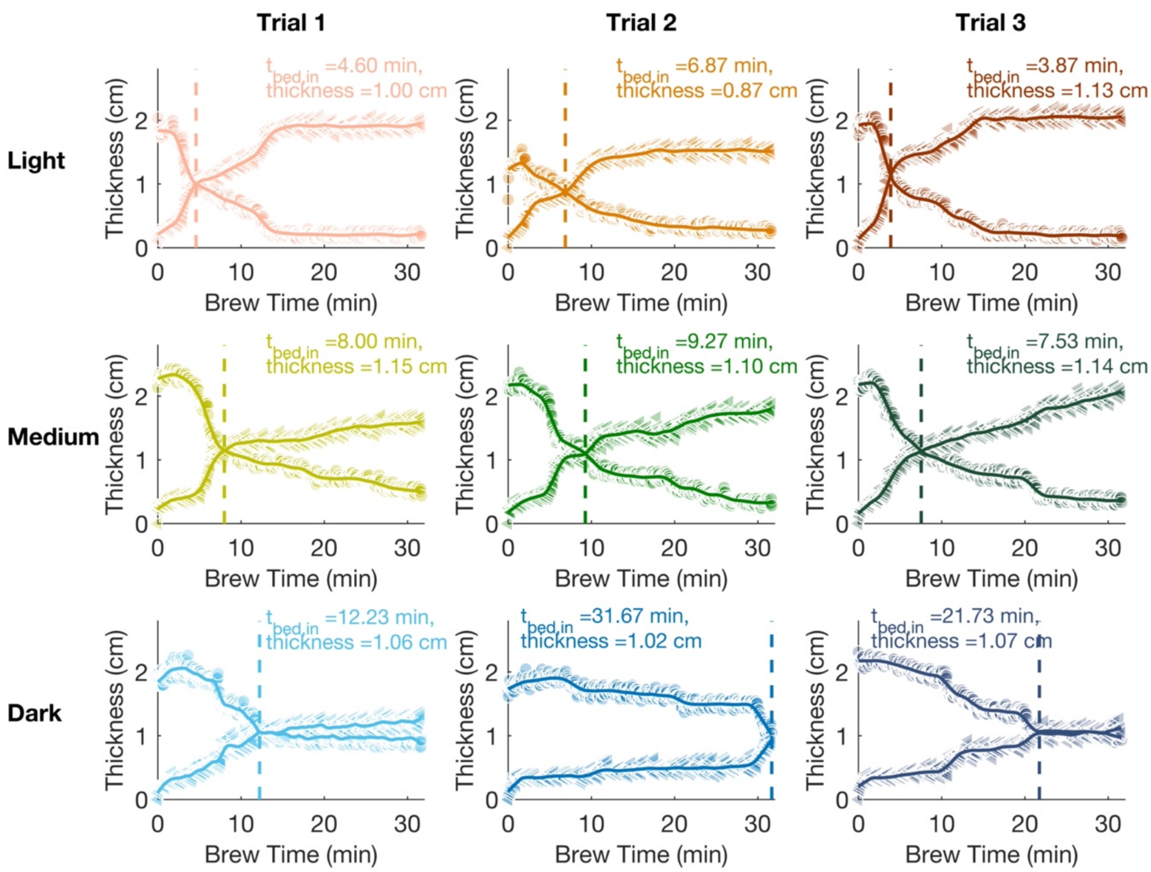


Figure 5-3. Scatter plots of the thickness of the coffee ground layers vs. time of full immersion 40-g brews at $R_{brew} = 15$ with coffee at three roast levels (light, medium, dark) brewed at 99°C. The thickness of top bed is denoted by circles, and the thickness of bottom bed is denoted by triangles. Each row represents a different roast level, and each column represents a different individual trial replicate (each of which are indicated by different arbitrary colors). The solid lines represent the running average of the respective thickness (cf. 2.5), and the vertical dashed lines indicate the bed inversion timepoints $t_{bed,in}$ where the bottom thickness first exceeds the top thickness.

These dynamics can be quantified using a "coffee ground bed layer inversion time point," denoted as $t_{bed,in}$ and defined as the time at which the thicknesses of the top and bottom layers become equivalent, i.e., $\delta_{top} = \delta_{bottom}$. This inversion time serves as a convenient indicator of the characteristic sedimentation time scale for the coffee grounds (vertical dashed lines in Fig. 5-

3). Notably, the lighter roast coffee grounds sediment faster than the medium or darker roast coffee grounds. The $t_{bed,in}$ for light roast ranged from 3.8 min to 6.8 min, while for medium roast and it ranged from 7.5 min to 9.3 min. For dark roast, in contrast, the variation was much larger between trials, with $t_{bed,in}$ varying from 12.2 min to the entire observation period (more than 30 min). Similar trends were observed with the larger 60-g brews (Supplementary Fig. 5-S3).

Furthermore, the averaged sum of the thicknesses of top and bottom layers, $\delta_{top} + \delta_{bottom}$, were (2.05 ± 0.20) cm, (2.26 ± 0.16) cm, and (2.19 ± 0.15) cm, for the 40-g brews with light, medium, and dark roast coffee, respectively, where each quantity represents the mean and standard deviation. The amount of coffee grounds was conserved within the brew, and the total thickness of the layers remained stable (to within about 10% accuracy) throughout the entire brewing period. Considering that the total thicknesses could be affected by swelling after immersion in water and off-gassing during brewing, the observed stability of the total grounds thickness suggests that such effects are minor.

To quantify more precisely the dynamics of the sedimentation process of coffee grounds, the sedimentation ratio was calculated from the thicknesses of the top and bottom layers coffee grounds using Equation (5-1) over the entire brewing period (Fig. 5-4). The overall trend is coffee brews with lighter roast asymptotically approach 85 to 90% sedimentation ratio, the medium roast approached 75 to 85% sedimentation ratio, and the darker roast approached only 45 to 55% sedimentation ratio. In other words, the lighter roast coffee grounds not only sedimented much faster but a much larger portion of the coffee grounds actually reached the bottom of the container by the end of 30 min. More specifically, at $t = 1\ min$, the average sedimentation ratios are 14.33%, 11.39%, and 11.92% for light, medium, and dark roast, respectively; at $t = 15\ min$, the average sedimentation ratios had increased to 83.90%, 63.97%, and 28.35%; and at $t = 30\,min$, the sedimentation ratios had reached 89.36%, 81.14%, and 43.74%. Notably, the sedimentation ratio was 51% higher in light roast compared to dark roast. Comparison between the 40-g brews and the 60-g brews indicated the larger batch size yielded a much more rapid increase in sedimentation ratio at a given roast level (Fig. 5-4B). For example, the medium roast coffee in 60-g brews reach 50% sedimentation in 3 to 4 min, but it required up to 10 min to reach the same sedimentation ratio in 40-g brews. Similar trends are observed at the other roast levels.

A final important observation regarding the sedimentation dynamics is that sudden increases in the sedimentation ratio were observed in all roast levels of the 60-g trials. These rapid increases happened within 5 min for the light and medium roasts and between 10 to 15 min for dark roast, with larger variability in the time of the increase between trials. We observed that occasionally after pipet sampling from the brew, an outflow of bubbles would suddenly escape from the top layer near where the pipette poked through (cf. Supplementary Video 5-S4). These bubbles apparently accumulated under the crust until a rapid bubble outrush off-gassing occurred, followed by a sudden increase in sedimentation. We emphasize that the pipette was 'poking' the crust many times prior to the bubble outrush, so it is unclear why any particular pipet sampling event would cause the bubbles to suddenly escape. The subsequent increase in sedimentation rate is presumably due to a decreased amount of gas helping keep the coffee grounds buoyant.

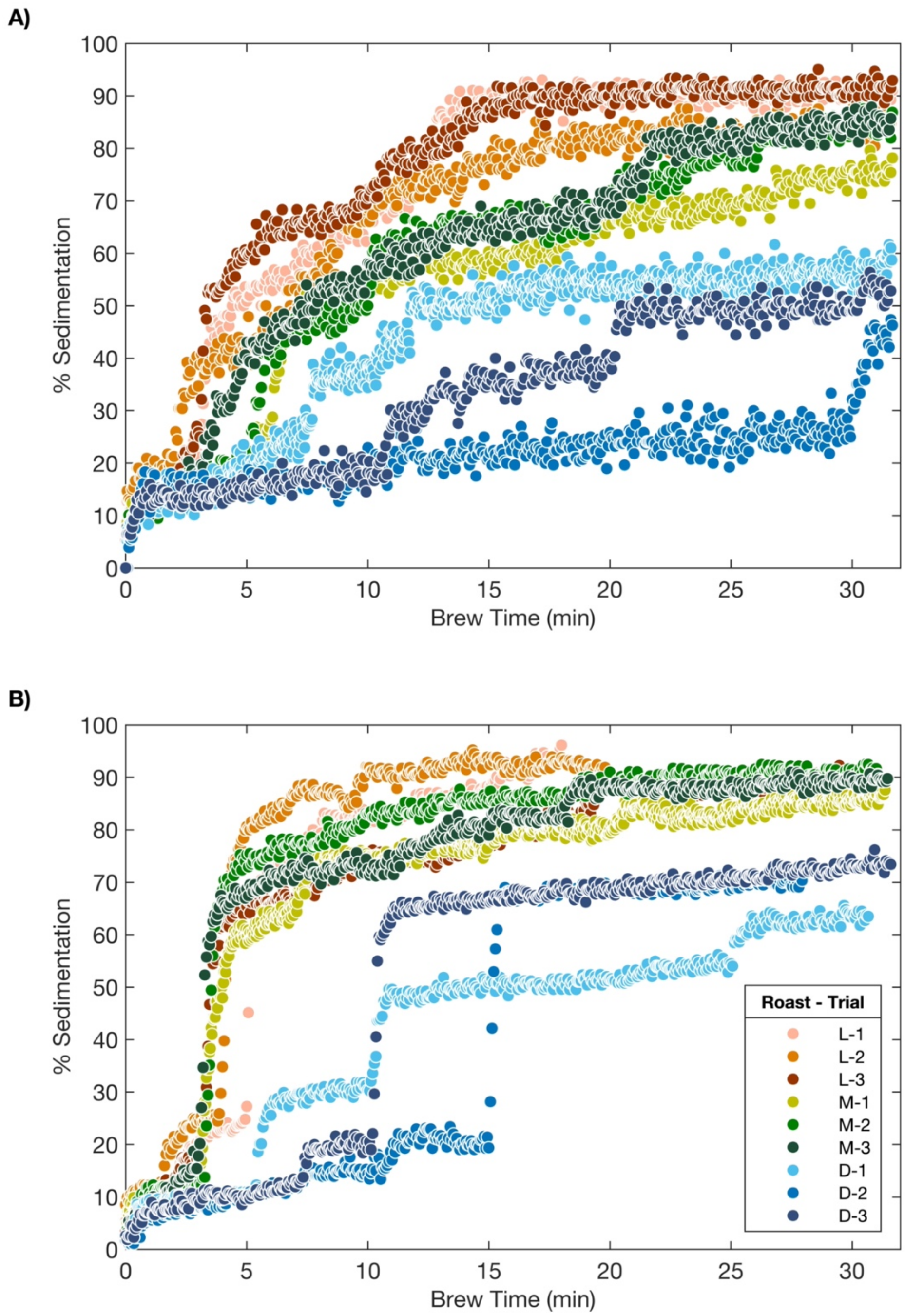


Figure 5-4. Scatter plots of the sedimentation ratio (cf. Eq. 5-1) vs. time for (A) 40-g and (B) 60-g full immersion brews at three roast levels (light-L, medium-M, dark-D), all brewed at 99°C. Colors for each trial are the same as in Figure 5-3.

5-4.2 Concentration Gradient over Time

The key goal of this study was to determine how the sedimentation dynamics shown in Figs. 5-2 and 5-3 affect the spatiotemporal dynamics of extraction of the coffee grounds into the liquid phase. The *TDS* sampled at different depths and times within the brew is shown in Figure 5-5, where the same data are presented in two different fashions: organized by roast level (Fig. 5-5A) and organized by depth within the brew (Fig. 5-5B). At a given roast level, the *TDS* of samples taken from the surface of the brew (depth = 0 cm) was initially two times higher, approaching 3%, while the *TDS* sampled from other positions remained below 1.5% in the first 3 min at all roast levels (Figure 5-5A, light pink circles, light green triangles, and light blue squares, respectively). As time progressed, the *TDS* at 0 cm generally decreased toward a constant value between 1 to 1.4% depending on roast level. In contrast, the *TDS* at lower depths tended to start at much lower values, near 0.6%, and then increased with time. This means that a *TDS* spatial gradient inversion occurred: initially the highest concentration was at the top (near 0 cm), but then the highest concentration was near the bottom (8 cm).

A notable feature of the data is that the *TDS* sampled from the top-middle of the brew (depth = 2 and 4 cm) are much more consistent with each other at all roast levels, such that they vary more smoothly in time with an average and standard deviation of $(1.21 \pm 0.09)\%$ within the time period from 10 to 60 min, compared to the much higher *TDS* values at the bottom of the brew (depth = 6 and 8 cm) which exhibited tremendous scatter with an average and standard deviation of $(1.92 \pm 0.44)\%$. After $t = 10$ min, the *TDS* sampled from the bottom of the brew (8 cm) reached a concentration twice as high compared to the top or middle of the brew for light and medium roasts. In addition, the variations in *TDS* between samples from the top and bottom positions was larger in the light and medium roasts than dark roast within the 30-minute brewing period. For example, the ranges of concentration (*TDS*) gradient at $t = 20$ min are 1.42% in light roast, 1.28% in medium roast, and 0.40% in dark roast, where these values are the average range of *TDS* across trial replicates measured between depth = 0 cm and 8 cm.

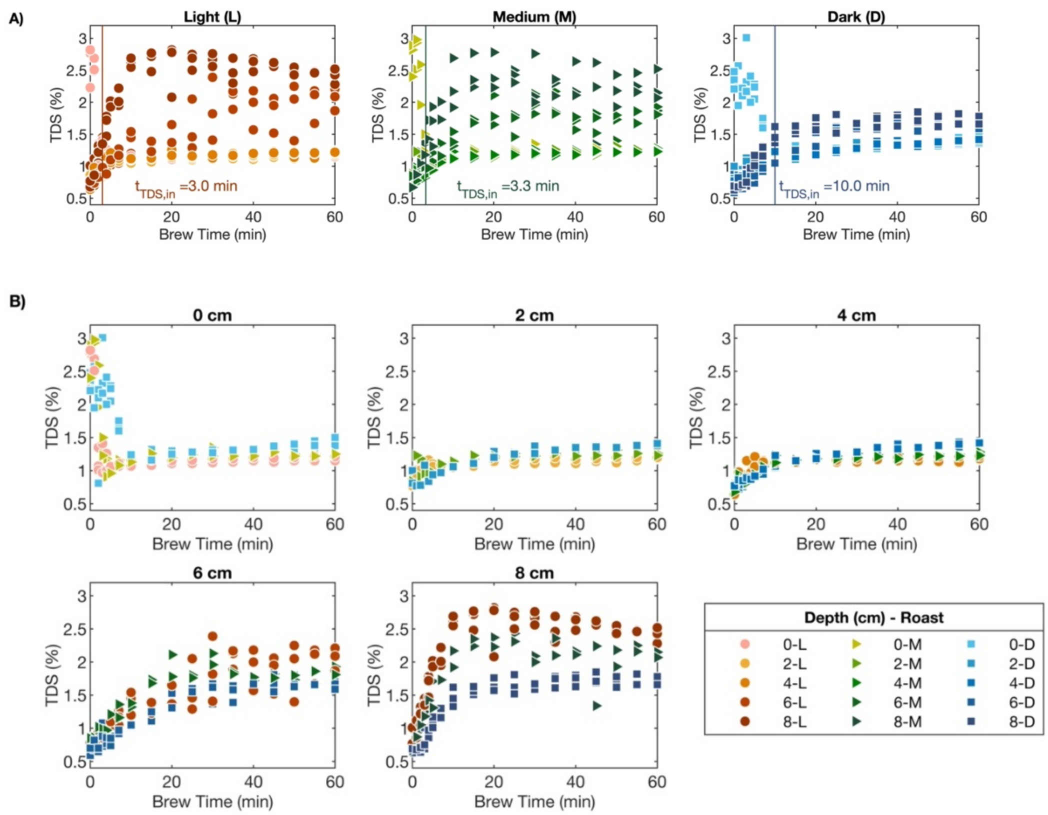


Figure 5-5. Scatter plots of the dynamic *TDS* sampled at various sampling depths below the surface for 40-g full immersion brews at $R_{brew} = 15$ with coffee at three roast levels (light-L, medium-M, dark-D), all brewed at 99°C. (A) and (B) show the same data organized by roast level or sampling depth, respectively. Different roast levels are indicated by different shapes, different depths are indicated by different colors. The vertical lines represent the average *TDS* inversion timepoint $t_{TDS,in}$, which is the first time point at which the *TDS* sampled at the surface (0 cm) became smaller than the *TDS* sampled at the bottom of brew (8 cm). Note the color scheme here differs from the color scheme used in Figures 5-3 and 5-4.

Furthermore, at a given sampling position of the brew, roast level also influenced *TDS* at the extreme sampling positions (Figure 5-5B). At the surface of the brew (depth = 0 cm), *TDS* of dark roasts remains higher than the final plateau value in the first 5 min, while the *TDS* of light and medium roast quickly decreased within the first 3 min. At the bottom of the brew (depth = 8 cm), the dynamic *TDS* values are consistently the highest in light roast, and lowest in dark roast during the entire brewing period. However, such trends are not obvious in the middle positions (depth = 2, 4, and 6 cm). Furthermore, *TDS* values were more consistent between trial replicates when sampled from the 2 and 4 cm positions than the 6 cm position.

5-4.3 Correlation of Sedimentation and Concentration Gradient

Our central hypothesis is that the concentration gradients in the brew are governed by the coffee ground sedimentation time scale. To test whether the sedimentation dynamics and concentration gradient inversion dynamics are correlated, we performed a correlation analysis between the *TDS* at three different depths (surface – 0 cm, middle – 4 cm, and bottom – 8 cm) and the corresponding thicknesses of both the top and bottom coffee ground bed layers across all roast levels (Fig. 5-6). The correlations presented in Figure 5-6 are all statistically significant. The *TDS* sampled at the surface is positively correlated to the top coffee bed thickness (Fig. 5-6A), but negatively correlated to the bottom bed thickness (Fig. 5-6B); contrariwise, *TDS* sampled in the middle and at the bottom of the brew is negatively correlated to the top coffee bed thickness (Figs 5-6C and 5-6E), and positively correlated to the bottom bed thickness (Figs. 5-6D and 5-6F).

The *TDS* sampled at the bottom of the brew (8 cm) had the strongest correlations to the thicknesses of both top and bottom coffee bed layers: the correlation coefficients are -0.933 with the top layer and 0.972 with the bottom layer. In other words, as brewing proceeds, the concentration of soluble solids near the bottom of the brew increased in direct proportion to δ_{bottom}. In contrast, *TDS* sampled at the surface had the weakest correlation with any of the thicknesses of coffee bed layers, with correlation coefficients of 0.624 and -0.692 respectively. The weaker correlations are presumably due to the high *TDS* presence in at the surface of the brew in the very beginning period of the brew, which appears to be rigidly step, followed by relatively constant *TDS* measurements over time. The *TDS* sampled from the middle position (4 cm) also has weaker correlation with the coffee bed layers than the 8-cm ones, and remained the most consistent in *TDS* measurement over time compared to other sampling positions.

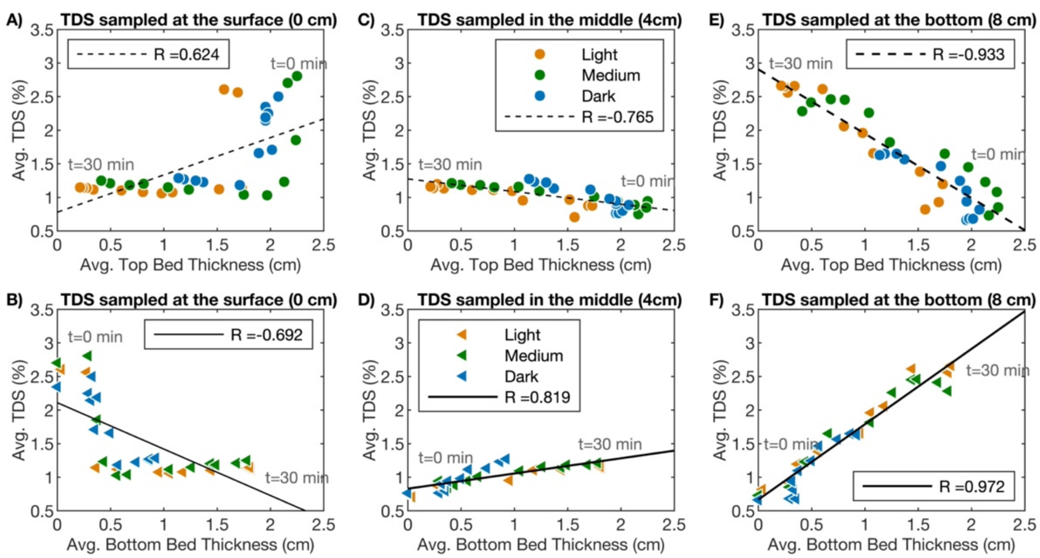


Figure 5-6. Scatter plots of the average *TDS* sampled at the surface (A & B), the middle (C & D), and the bottom (*E* & F) of the beaker vs. the average thickness of the coffee ground bed measured on top (A, C, E) and bottom (B, D, F) for the 40-g full immersion brews. Different roast levels are indicated by different colors. Each point represents an average of three trial replicates. The thickness of the top bed is denoted by circles, and the thickness of the bottom bed is denoted by triangles. The best fit lines through the data points are also plotted along with the corresponding correlation coefficients.

Furthermore, our findings also suggest that the *TDS* inversion time points is related to the coffee bed layer inversion time points. Correlation and regression analyses were performed between the *TDS* inversion time points $t_{TDS,in}$ (vertical lines in Fig. 5-5A) and the coffee bed layer inversion time points $t_{bed,in}$ (cf. Figure 5-3) at the three different roast levels. The resulting scatter plot with three data points is shown in Supplementary Figure 5-4. Consistent with the qualitative observations, we find that the *TDS* inversion timepoint and coffee bed thicknesses are positively correlated to each other with a correlation coefficient of 0.993, suggesting that the concentration gradient inversion present in the brew is positively correlated to the process of sedimentation. The p-value, however, is 0.0744, reflecting the sizable error bars reflecting the large variability in the two inversion time scales, especially in dark roast. The inversion timepoints of dark roast are significantly different than light or median roast as their error bars do not overlap, where the difference between light and medium roast is not as pronounced. To put this point on a statistically rigorous basis, further experimentation with trial replicates at more than three roast levels will be needed.

5-5. Discussion and Conclusions

Taken together, our data indicates that a seemingly "quiescent" full immersion brewed coffee is a highly heterogeneous mixture, in which the concentration (*TDS*) of liquid coffee differs depending on both time and the specific position within the brew. The magnitude of the concentration gradient varies over time, with a region of nearly twice as high concentration near the surface in the beginning, then a more than twice as high concentration region eventually developing near the bottom as the brewing and sedimentation proceed.

5-5.1 Concentration Gradient, Diffusion, and Sedimentation

Previous work on extraction in full immersion coffee brewing has focused on diffusion processes in a well agitated system (Moroney et al., 2016; Spiro, 1993; Spiro and Selwood, 1984; Zanoni et al., 1992). In the absence of external agitation, however, our findings imply that the concentration gradient in the unagitated brew is caused by sedimentation of the coffee grounds, with the highest *TDS* located at the depth where the coffee particles are most concentrated. The resulting vertical concentration gradient will engender diffusion down the gradient, but the timescale of purely diffusional transport is extremely slow compared to the sedimentation time scale. The diffusive time scale can be estimated as

$$t_{dif} \sim \frac{L^2}{D}, \qquad (2)$$

where L is the characteristic height of the brew and D is a characteristic diffusivity of a soluble species in water. A representative coffee soluble is caffeine, which in aqueous solution has a diffusion coefficient of approximately $2.0 \times 10^{-9}\ \mathrm{m}^2/s$ at 80°C (Jaganyi and Madlala, 2000; Price, 1989; Spiro et al., 1989; Spiro and Hunter, 1985). The average heights of our 40-g brews over the 30-minute brewing period are 7.1 cm, 7.8 cm, and 8.0 cm for light, medium, and dark roast, respectively, so t_{dif} is estimated to be on the order of 10^6 s (almost 300 h). In contrast, our experimental data showed that an inversion of concentration gradient is observed within half an hour. Thus, the spatial concentration gradients of coffee solubles form and rearrange too quickly to be explicable solely via diffusion, considering the diffusion time scale is in the order of 10^6 s; instead, the data indicate that the concentration gradients in full immersion coffee brews are determined primarily by the sedimentation behavior of the particulates and the local diffusional mass transfer out of the particle interiors into the local fluid. A more precise analysis will require consideration of other factors that affect the concentration gradient and coffee grounds sedimentation, including particle size distribution (Uman et al., 2016), chemical composition of coffee beans at different roast levels (Wei and Tanokura, 2015), natural convection within the brew caused by differences in local solution density, and thermal properties of the brewing container, which affects the rate of cooling and concurrent sedimentation processes, should also be considered and needs future exploration.

5-5.2 Density of Coffee Grounds and Sedimentation

Another important finding from our study is that dark roast coffee sediments slower than lighter roast coffee. Our density measurements showed that the bulk density of loose and tapped coffee grounds decreases with roast level (Table 5-1). In other words, at a fixed grind size, lighter roast coffee grounds are denser than darker roast coffee, which is consistent with previous studies (Nakilcioğlu-Taş and Ötleş, 2019; Ortolá et al., 1998; Schenker et al., 2000). The density of coffee grounds is known to change when they are wetted due to swelling of coffee particles, but previous work has found that the degree of swelling is independent of roast level (Hargarten et al., 2020). A slower sedimentation velocity for dark roast is therefore expected based on the decreased density. A potential confounding factor, however, is that a lower density of the coffee grounds for a given average particle size suggests a higher porosity, and increased porosity is known to alter sedimentation velocities (Emadzadeh and Chiew, 2020). Additionally, the release of CO_2 off-gassing during brewing also affects the sedimentation as it contributes to the buoyancy of the top layer of coffee grounds. Prior studies have found that the residual CO_2 content in coffee after grinding depends on roast level, and the rate of CO_2 off-gassing depends on both grind size and roasting temperature (Smrke et al., 2018; Wang and Lim, 2014). Because of the higher residual CO_2 content in darker roast coffee grounds, the slower sedimentation rate in dark roast could be possibly due to the release of more CO_2 during brewing. Therefore, the observed difference in sedimentation speed is potentially due to a combination of changing density, porosity, and behavior of CO_2 off-gassing during brewing. Future experimentation would benefit from in *situ* measurements of the CO_2 levels above the brew to characterize the off-gassing dynamics and their correlation with sedimentation and concentration gradient inversion.

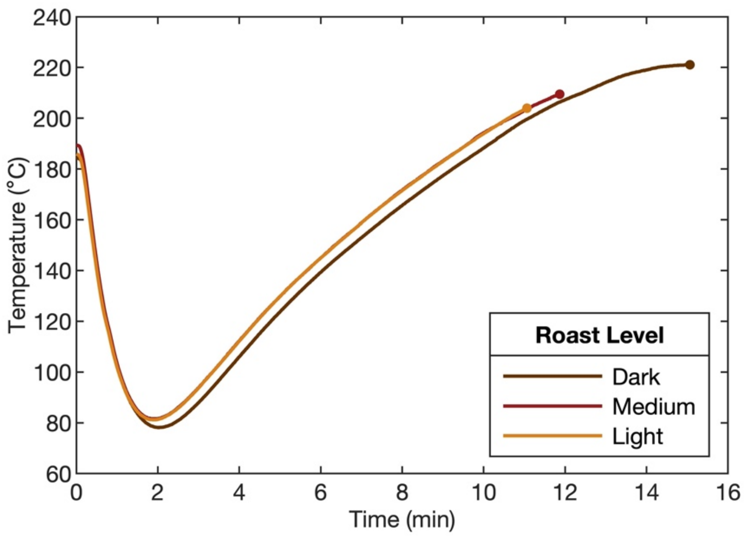
5-5.3 Implications for Sampling of TDS

An important implication of the concentration gradient inversion is that it tremendously complicates interpretation of *TDS* measurements for non-agitated full immersion brews (like French press or the traditional cupping procedure). Because the brew is heterogenous, the sampling position matters. Sampling from the top or bottom of the brew will either overestimate or underestimate the overall brew strength at different sampling time points. For example, sampling from the bottom of the brew at 2-minutes brew time underestimates the brew strength but overestimates the brew strength at 20 min. That is, the measured *TDS* will depend strongly on how deep the pipette is inserted. However, our results indicates that sampling from the middle of the brew (2 to 4 cm below the air/liquid surface) yielded consistent *TDS* values over the entire brewing process of 30 min that were representative of the average *TDS* within the brew (Figure 5-5B). In other words, researchers investigating the *TDS* of full-immersion coffee should be careful in non-agitated brews to always sample from the same depth near the middle of the brew.

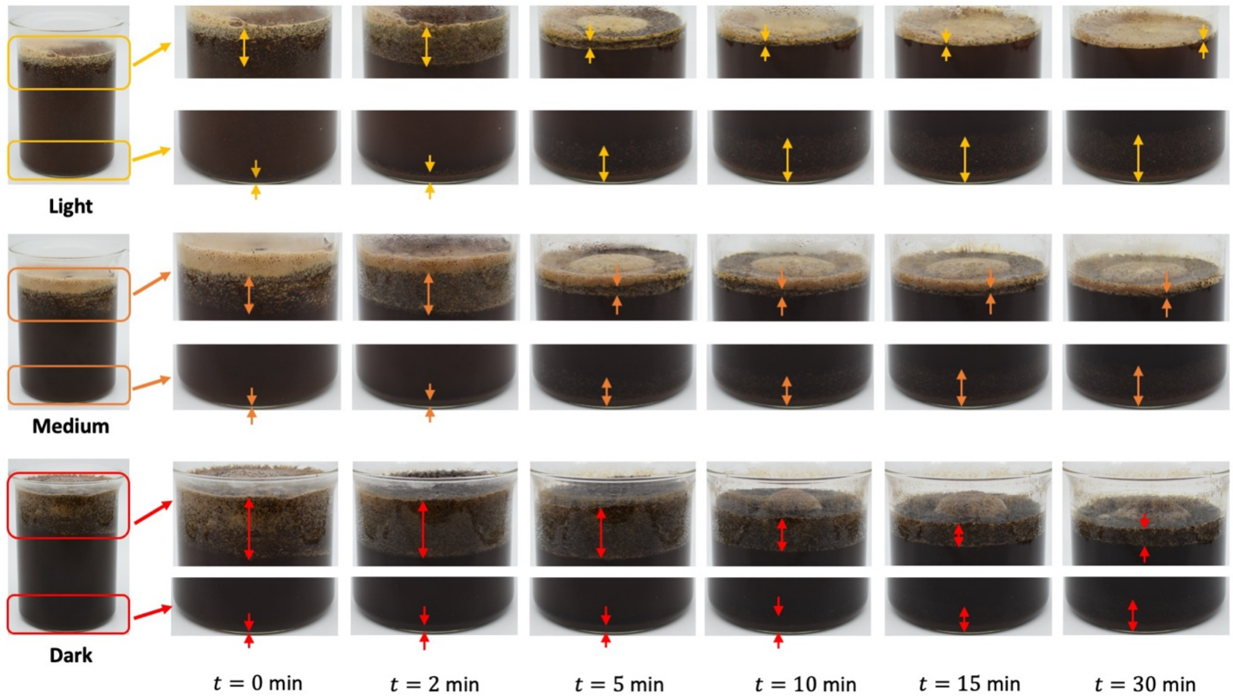
5-5.4 Implications for Full Immersion Coffee Brewing Practitioners

Our results have several practical implications to full immersion coffee brewing practitioners, especially in coffee cupping, which is mostly non-agitated with the only minor agitation as breaking the crust and skimming on the surface of the brew. Our work evaluated the consistency of *TDS* for cupping coffee beans from different roast levels. Typically, coffee cupping sessions include coffee beans from different roast levels in practical scenarios when multiple coffee beans are assessed at the same time. The entire cupping coffee brewing process from blooming, breaking the crust, and skimming generally takes 11-15 min before the tasting begins. During tasting, coffee cuppers use a spoon to scoop from the surface of the brew to assess specific flavor attributes of coffee (Lingle and Menon, 2017). It is well established that the sensory quality and consumer acceptance of coffee is highly associated with *TDS* (Batali et al., 2020b; Cotter et al., 2021; Frost et al., 2020), so examining the sensory characteristics of coffee under a controlled *TDS* is crucial. Based on our findings, coffee sampled from the surface brew from 10 to 60 min reaches a consistent *TDS* at a fixed roast level (Figure 5-5B), where the mean and standard deviation of the surface *TDS* are $1.15 \pm 0.04\ \%$ for light roast, $1.22 \pm 0.05\ \%$ for medium roast, and $1.31 \pm 0.08\%$ for dark roast. Even at the same *TDS*, however, differences in the chemical composition of coffee at different roast level might also affect the extraction dynamics and maximum extractability (Batali et al., 2022; Córdoba et al., 2021; Moroney et al., 2015; Rao et al., 2020), and thus alter the specific concentration and flavor profiles observed in a given brew. Coffee cupping practitioners should be aware of the natural variations in *TDS* caused by the difference in roast levels even when the coffees are brewed following identical protocols and tasted at the same time.

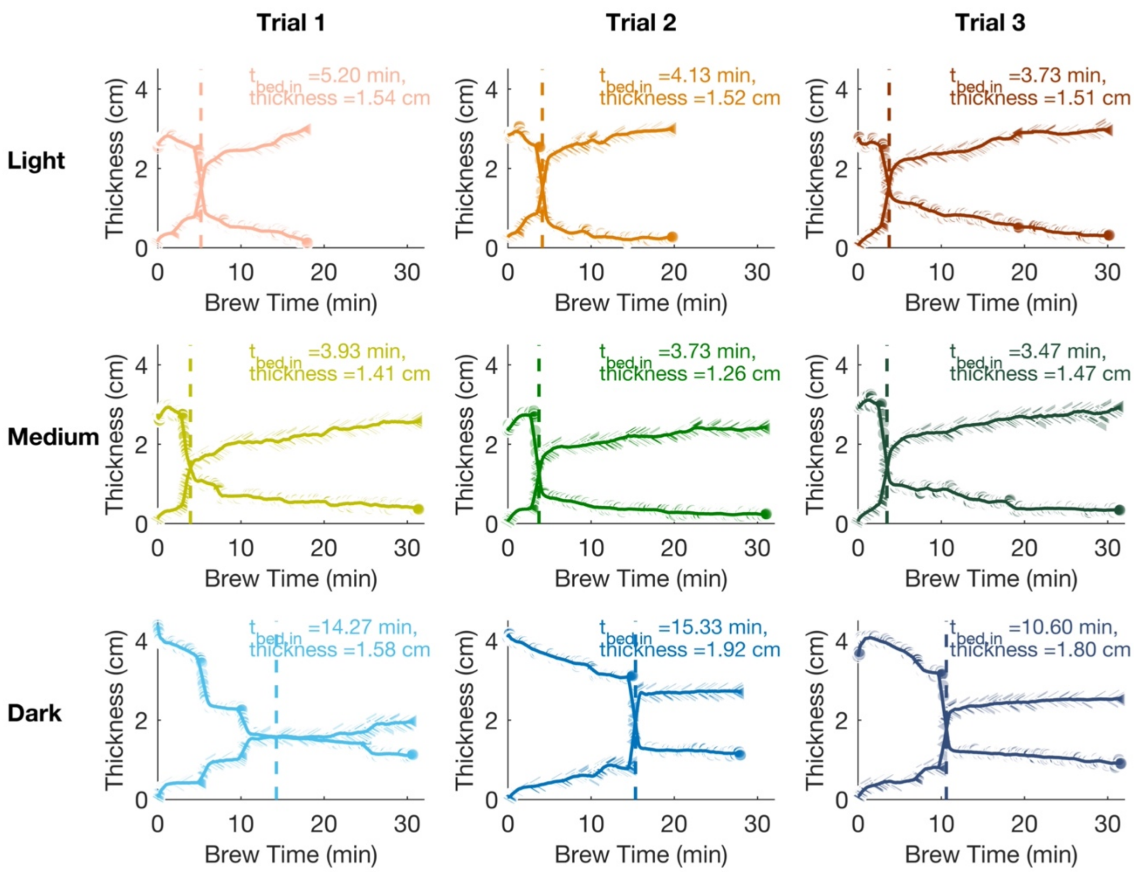
Supplementary Materials



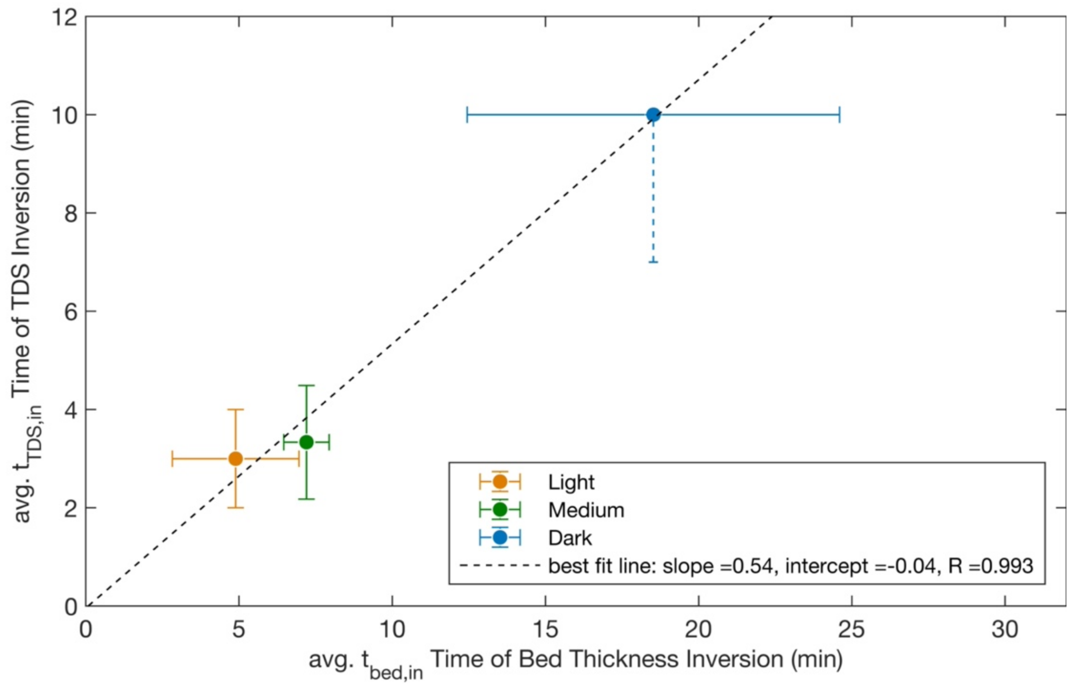
Supplementary Figure 5-S1. Roast profiles of the coffees used in the experiment. Because the light and medium roast profiles partially overlap, the end points of different roast profiles are denoted with circle to highlight the differences.



Supplementary Figure 5-S2. Representative images of full immersion 60-g brews with light, medium, and dark roast coffee at 0, 2, 5, 10, 15, and 30 min of brew time. The thickness of coffee ground beds at top and bottom are indicated by arrows.



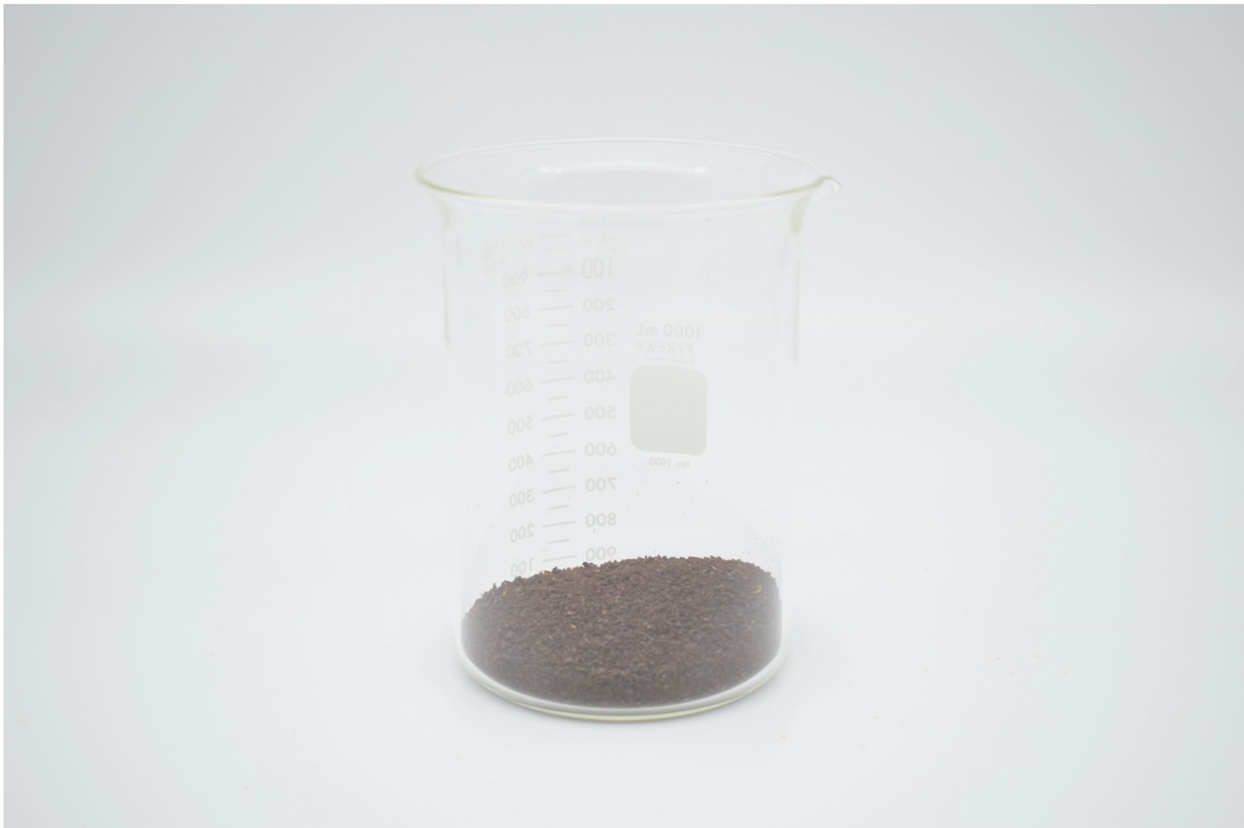
Supplementary Figure 5-S3. Scatter plots of the thickness of coffee ground beds vs. time of full immersion 60-g brews at $R_{brew} = 15$ with coffee at three roast levels (light, medium, dark) brewed at 99°C. The thickness of top bed is denoted by circles, and the thickness of bottom bed is denoted by triangles. Different roast levels are indicated by different color groups, different individual trials are indicated by different colors. The vertical lines represent the bed thickness inversion timepoints $t_{bed,in}$ where the first absolute minimum of difference in thicknesses of top and bottom bed is found.



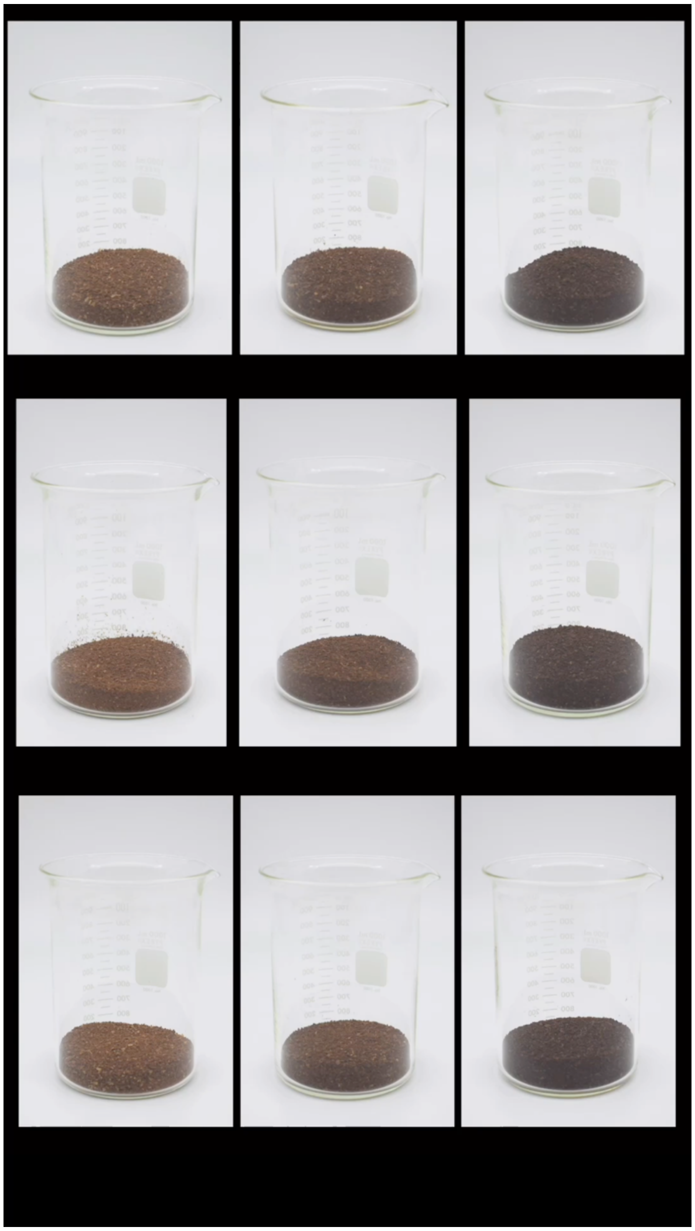
Supplementary Figure 5-S4. Scatter plot of the average *TDS* inversion timepoint $t_{TDS,in}$ vs. the average bed thickness inversion timepoint $t_{bed,in}$ for 40-g brews (cf. Figs 3 and 5). Different roast levels are indicated by different colors. The solid line error bars indicated by colored lines are the standard deviation between trial replicates, and the dashed vertical error bar of dark roast is illustrated by measurement error. The vertical error bar on dark roast is one-sided because it is illustrated by the uncertainties in measurement errors when the inversion time did happen somewhere between two consecutive time points where *TDS* were sampled at 7 min and 10 min. The best fit lines through the data points are also plotted along with the correlation coefficients of $t_{TDS,in}$ and $t_{bed,in}$.

Supplementary Video 5-S1. Time-lapsed video for a representative 40-g full immersion brew with light roast coffee.

Supplementary Video 5-S2. Time-lapsed video for a representative 40-g full immersion brew with medium roast coffee.



Supplementary Video 5-S3. Time-lapsed video for a representative 40-g full immersion brew with dark roast coffee.



Supplementary Video 5-S4. Time-lapsed videos for 60-g full immersion brews. Trials with light, medium, and dark roast coffees are in the left, middle, and right columns, respectively.

Chapter 6. Sensory analysis of the flavor profile of full immersion hot, room temperature, and cold brewed coffee over time

---

Author Contributions:

Jiexin Liang co-designed the study, conducted experiments, performed data analysis and figure preparation, and wrote the original draft of the manuscript. Mackenzie E. Batali co-designed the study, conducted the experiments, and edited the manuscript. Catherine Routt conducted experiments. William D. Ristenpart and Jean-Xavier Guinard secured funding, co-designed the study, advised data analysis, revised and edited the manuscript.

6-1. Abstract

With the growing popularity of cold brewed coffee comes a need for brewing efficiency while preserving the desirable flavor profile. Despite the wide use of full immersion brewing techniques, the effect of brew time on the dynamic sensory profiles of full immersion brewed coffee remains underexplored. Here, we investigated the relationship between coffee sensory quality and extraction dynamics, measured as Total Dissolved Solids (*TDS*) and Extraction (*E*) of full immersion brewed coffee at various roast levels, brewing temperatures (4°C, 22°C and 92°C), over brew time using a generic descriptive analysis method. Specifically, different brew time points were selected for different temperatures based on five targeted coffee extraction stages. Furthermore, the unique experimental design also explored a sensory-driven engineering research process.

Roast level had the greatest impact on the sensory profile of the coffees, followed by brewing temperature, but brew time, especially the longer brew times as *TDS* plateaued, had much subtler impacts than expected. Twenty-five of 28 sensory attributes were significantly different among the 30 coffee samples, indicating a single source green coffee blend can produce a wide range of complex sensory profiles using different combinations of roast level, temperature, and brew time. Specifically, the intensity of sweetness was negatively correlated with *TDS*, and 19 other attribute intensities were positively correlated with *TDS*. Interestingly, we found that that certain long time cold brews had similar sensory profiles to those of some short time hot brews, suggesting the sensory profiles of certain hot brews and cold brews could possibly be matched through controlled preparation. Overall, our study demonstrated an approach of integrating food engineering and sensory analysis for product development, and our findings

provide valuable insights into the extraction dynamics and sensory quality of full immersion brewed coffee and opens new brewing avenues for the coffee industry.

6-2. Introductions

The importance of *TDS* and *E* on sensory quality and consumer liking of coffee has been well established (Batali et al., 2020b; Cotter et al., 2021; Frost et al., 2020; Guinard et al., 2023; Lockhart et al., 1957). While most coffee sensory studies of brewed coffee focused on pressurized espresso brew or flow-based drip brew method (Batali et al., 2021, 2020a, 2020b, Frost et al., 2020, 2019; Gloess et al., 2013; Vezzulli et al., 2022), there are comparatively less sensory studies on full immersion brewing methods other than a few recent ones focused on cold brew (Angeloni et al., 2019b; Córdoba et al., 2021; Cordoba et al., 2019; Gloess et al., 2013; Seninde et al., 2020). The connection between sensory quality and extraction dynamics of full immersion brewed coffee under various brewing condition is also missing. Especially for coffee cupping, the coffee industry relies on the Specialty Coffee Association (SCA) standards and protocols as guidelines to prepare coffee samples (Lingle and Menon, 2017). However, the effects of brewing parameters effects on extraction dynamics in the cupping brewing process remain underexplored. The process of cupping involves tasting the coffee at multiple time points as coffee cools down throughout the entire brewing process (Lingle and Menon, 2017). However, no scientific study to date has systematically assessed the dynamic sensory profile behind full immersion brewed coffee in response to various brewing parameters, such as grind size, brew ratio, brew temperature, and roast level. Moreover, the difference in extraction dynamics in response to roast level also has crucial implications for sensory quality of full immersion brewed coffee: the sensory properties of coffees with different roast levels evaluated at the same time point under the same temperature could be confounded by the difference in strength (Liang et al., 2023, n.d.).

Therefore, the sensory quality of full immersion brewed coffee depends on multiple brewing parameters.

To understand the effects of roast level and key brewing parameters on the sensory quality of the brew, a combination of engineering and sensory evaluation approaches is needed to investigate how physical characteristics of the cup vary with controllable parameters, and how such measurable physical properties (*TDS* and E) correlate with sensory properties of full immersion brewed coffee. For the vast majority of coffee baristas and coffee consumers, the practical question of how to brew a cup of coffee with a desired sensory profile using full immersion brewing techniques has yet to be fully answered.

Our prior sensory analysis on the effects of origin, roast level, and brewing temperature on the flavor profile of full immersion brewed coffee at fixed equilibrium *TDS* and cold consumption temperature showed that brew temperature across the cold to hot range had a significant impact on the sensory properties of coffee, and that different roast levels and origins also yield differences in sensory attributes with temperature (Batali et al., 2022). Yet, this study eliminated the effect of total brew time that yields difference in final *TDS*, which is also a key factor in coffee cup quality (Liang et al., 2021, n.d.).

On the other hand, the coffee industry heavily relies on the full immersion method of "cupping" to evaluate coffee quality, mainly following the SCA standards and protocols (Lingle and Menon, 2017). Despite the widespread use of this procedure and the industry's continuous dedication to enhancing it (Specialty Coffee Association, 2022), there are questions remain about the consistency and effectiveness of this sensory evaluation process used in the industry (Di Donfrancesco et al., 2014; Fioresi et al., 2023; Pereira et al., 2017), and there is still a need of published scientific justification for the details of the protocol. We therefore wanted to answer the following questions: how does the sensory profile of the coffee cup change over time after water addition, as it continues to extract, and cools down to room temperature? How does this dynamic sensory profile change in response to different roast levels and brewing parameters? What are the relationships between the physicochemical measurements (*TDS*, pH, and TA) and the sensory quality of coffee over time? How do we design the sensory profile of immersion coffee via actionable brewing parameters?

To answer these questions, this study related the extraction dynamics to the sensory quality of full immersion coffee following a sensory-driven engineering approach. We explored the flavor profiles and investigated the effects of roast levels, brewing temperatures, and brew time on the sensory quality of full immersion brewed coffee using a generic descriptive analysis method in conjunction with *TDS*, TA, and pH measurements.

6-3. Methodology

6-3.1 Experimental Design

We used a 2 X 3 X 5 factorial design, with a Central America coffee blend roasted to 2 different roast levels, and each brewed at three different temperatures (4°C, 22°C, and 92°C), to five different time points that corresponded to five brewing stages from "rinse" to equilibrium of full immersion brews. Each of the 30 coffee samples were prepared in triplicate for both physical/chemical and sensory measurements. The physical/chemical properties of the coffee were measured as total dissolved solids (*TDS*), titratable acidity (TA), and pH, and the sensory properties of the coffees were evaluated using a generic descriptive analysis method.

6-3.2 Coffees

A South American blend coffee composed of an El Salvador Cerro Las Ranas coffee and a Nicaragua Parainema coffee were roasted to two different roast levels, representing a "light" roast, denoted by light roast (L), and a darker end of "medium-dark" roast, denoted by dark roast (D) (Coffee Review, n.d.). Roasting was done in a single day using a Probat Probatone P-5 roaster (Probat-Werkevon Gimborn Maschinenfabrik GmbH, Emmerich am Rhein, Germany) at the UC Davis Coffee Center. The average roast colors of the roasted beans were 71.8 and 41.8 for the light and dark roasts, respectively, measured using an Agtron Gourmet Color Scale (Specialty Coffee Association, 2018) (Agtron E2OCP-II Coffee Analyzer, Agtron Inc., Reno, NV, USA). Roasted beans were degassed for a week at room temperature, then vacuum-sealed in bags and stored in a freezer at −20 °C. To ensure consistent sensory quality, individual bags of coffee were defrosted at room temperature overnight before use.

6-3.3 Coffee Brewing

A schematic visualization of the brewing and serving process is shown in Figure 6-1. All roasted coffee beans were ground to a consistent grind size setting of 4, corresponding to a median particle size of $972 \pm 19\ \mu m$ (cf. Supplemental Figure 6-S1 in (Liang et al., 2021) reference in a classic Mahlkönig Guatemala Lab Grinder (Mahlkönig USA, Durham, NC, USA). Coffee from both roast levels were each brewed using water at three different temperatures: 4°C (typical temperature of refrigeration), 22°C (room temperature), or 94°C (within the range of suggested temperature for hot brewed coffee (Lingle, 2011)). The refrigerator and room brews were brewed for 0, 4, 8, 12, and 24 hours and the hot brews were brewed for 0, 4, 10, 30, and 60 minutes, each corresponding to time points denoted as T1, T2, T3, T4, and T5, respectively. Time points were chosen based on representative extraction stages of full immersion brews: T1 was the "rinsed" coffee, T2 and T3 were during and near finish of the rapid increase in *TDS*, and T4 and T5 were after the *TDS* of the brew had reached apparent equilibrium.

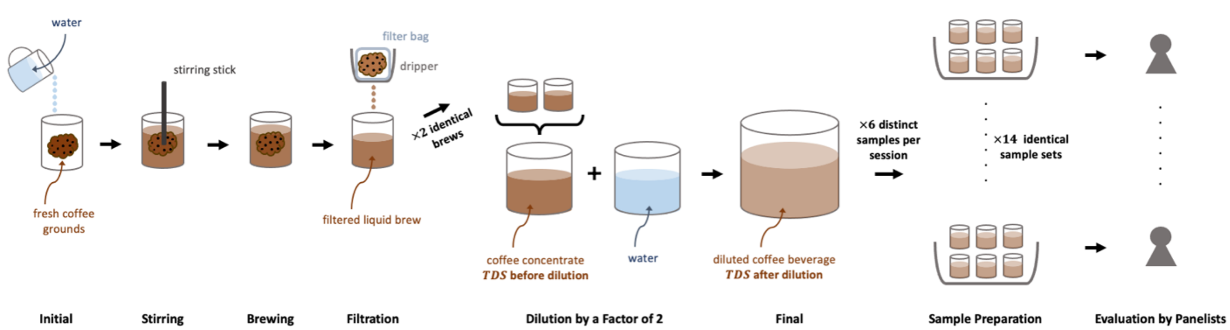


Figure 6-1. A schematic of coffee brewing and the sensory evaluation process.

All coffees were brewed using a full immersion brewing technique in Toddy Cupping Kits (Toddy LLC., Loveland, CO, USA) with Nestlé Pure Life Purified Water (Nestlé Waters North America, Inc., 2021) (Nestlé Waters North America Inc., Stamford, CT, USA) at a water-to-coffee brew ratio $R_{brew} = 5$, which is a typical brew ratio the industry uses for cold brew concentrate (Toddy, 2020). For the refrigerator temperature brews, water was pre-refrigerated to 4°C; for the room temperature brews, water temperature was set at 22°C; for the hot brews, water was heated to 92°C using a Bonavita 1.7-L Variable Temperature Electric Kettle (Bonavita World, Woodinville, WA, USA). All coffees were brewed using the following full immersion technique: First, 100 g of coffee grounds were measured and placed into the glass container, and 500 g of water at target temperatures (4, 22, or 94°C) was poured into the beaker using a goose-neck kettle in circular pouring motion. The timing of the brew started upon completion of the water pouring. Then, the coffee brew was stirred using a stirring stick for 15 seconds to ensure all coffee grounds were fully wet. After that, the brew was covered by lid and brewed to designated brew time. During brewing, the fridge brews were stored in a refrigerator at 4°C, while the room and hot brews were placed on a wooden countertop at room temperature. When the brew reached the designated brew time, the entire coffee brew was filtered through a filter paper to separate the liquid coffee brew from the coffee grounds. Two identical brews were conducted per brewing conditions. The resulting coffee liquid brew from the identical brews were combined into a coffee concentrate, in which a 2mL sample was drawn using a disposal pipet for *TDS* measurements. Then, the coffee concentrate was diluted with room temperature water by a factor of 2 by mass to obtain the diluted coffee beverage. A 100mL sample was collected from the coffee beverage for physical/chemical measurements, and the rest of the diluted coffee beverage was stored at

4°C overnight before sensory evaluation on the next day. All brewed coffee samples were performed with three trial replicates.

6-3.4 Physical and Chemical Measurements

The total dissolved solids (*TDS*) were measured for both the coffee concentrate before dilution and the coffee beverage after dilution at room temperature using a VST LAB Coffee III digital refractometer (VST Inc, Boston, MA, USA). The refractometer was calibrated according to procedures outlined in prior study (Liang et al., 2021). The corresponding extraction yield, *E*, was calculated form the measured *TDS* and R_{brew} using the following equation (Liang et al., 2021):

$$E = \frac{TDS}{1-TDS} R_{brew}. \tag{6-1}$$

The pH and titratable acidity of the coffee beverage after dilution were also measured at room temperature using a Mettler Toledo S220 SevenCompact™ Benchtop pH/IS*E* Meter (Mettler Toledo, Greifensee, Switzerland). The pH measurements were taken while the sample was stirred using a magnetic stir bar. Then, while the coffee was stirred, the titratable acidity was measured by adding 0.1 M NaOH (Sigma Aldrich, St. Louis, MO, USA) dropwise from a burette, until the solution reached a pH of 8.20 ± 0.01. Titratable acidity is expressed in mL NaOH/50 mL coffee. The pH meter was calibrated using acidic (pH 4.00 ± 0.01, color coded red), neutral (pH 7.00 ± 0.01, color coded yellow), and basic (pH 10.00 ± 0.01, color coded blue) calibration standards (VWR chemicals, VWR international, Radnor, PA, USA) before every set of six measurements. Physical/chemical measurements were conducted in three trial replicates consistent with sample tasted in descriptive analysis.

6-3.5 Descriptive Analysis

The training and sensory evaluation protocols were adapted from a generic descriptive analysis in accordance with amended IRB protocol 1082569-2. The panel was composed of 14 panelists, including 10 females and 4 males. In the Fall of 2021, ballot development and training were conducted in a group setting over nine 1-hr training sessions, where panelists tasted coffees and engaged in free term generation, drawing inspiration from the Coffee Taster's Flavor Wheel (Spencer et al., 2016). Following the selection of 27 attributes, panelists engaged in additional discussions and training to come to consensus and familiarize themselves with reference standards for all attributes incorporated in the final ballot. During the last week of training, panelists received reference materials alongside coffee samples, allowing them to work directly with the references while tasting coffees. All the attributes on the ballot are listed along with reference standards in Supplementary Table 6-S1. Before the actual evaluations, panelists conducted two mock sessions with a subset of the coffees to ensure alignment among panelists.

For the actual sensory evaluation, panelists participated in 15 tasting sessions, assessing 6 coffees per session. The evaluations were conducted in temperature-controlled, red-lit sensory booths to ensure panelists were isolated and not influenced by visual differences among the coffees. Samples were assigned a 3-digit random code and presented in a randomized Williams Latin Square block design to mitigate carryover effects. Coffees were presented to panelists one at a time, with a 2-minute interval between each sample. Data collection was conducted on RedJade (RedJade, Redwood City, CA, USA), where participants rated each attribute on an unstructured line scale ranging from 0 to 100, with anchor points at 10 and 90 labeled only with the words “Low” and “High”. Each coffee was evaluated in triplicate by the panelists on separate days. Coffee samples were served in white ceramic mugs containing 50 mL of coffee. To maintain a consistent consumption temperature for all panelists, coffee samples were served cold around 6°C and gradually warmed to around 12°C within 3 minutes during the tasting. Unsalted saltine crackers, water, and an empty cup for expectoration were provided to all panelists.

6-3.6 Data Analyses

Descriptive analysis data were exported from the data collection software, and ratings on the unstructured line scales were converted to scores from 0 to 100 for each attribute. All statistical analyses were conducted using RStudio 2022.07.1 Build 554. To understand the sensory characteristics of the coffee samples, Multivariate Analysis of Variance (MANOVA) across all attributes and Analysis of Variance (ANOVA) of individual attributes were used to determine which attributes were significantly different across the set of coffees. A three-way MANOVA (Product, Judge, Replication as factors) with two-way interactions using Type III sums of squares (SS) was used to analyze all the attributes at 5% significance level. The Wilk's Lambda test was used in MANOVA. Following a significant MANOVA result, univariate three-way ANOVAs with two-way interactions on each attribute were conducted with Type III sums of squares at the same significant level. For any attribute, if the main product effect was significant, and a Product*Judge or Product*Replication effect was significant in the univariate ANOVA result, then a pseudo-mixed ANOVA using the mean square of corresponding interaction effect as the error term was used to test the main product effect. Then, a five-way MANOVA (Roast, Origin, Temperature, Judge, Replication as factors) with up to three-way interactions using Type III sums of squares (SS) was used to analyze all the significant attributes at the same significance level. Attribute means determined to be significant for the experimental factors, including the ones from judge or replication effect by pseudo-mixed ANOVA, were then compared using Fisher's Least Significant Difference (LSD) in the "agricolae" package.

Principal Component Analysis (PCA) based on the significant attribute means were used to visualize of the sensory profiles of the 30 coffee samples. A correlation PCA was conducted using the "SensomineR" package, and PCA biplot was created using the "factoextra" package. The first three dimensions were investigated and interpretations were focused on the first two dimensions. In addition, a correlation PCA based on the raw attribute ratings data were conducted using Bootstrap techniques to display 95% confidence ellipses around products using the "SensoMineR" package. Pairwise comparisons of the products using Hotelling's T2 tests were also generated by the same function.

Correlation analysis between the intensity of sensory attributes and physical/chemical measurements was conducted, and the corresponding correlation plot was generated using the "corrplot" package. Furthermore, Multiple Factor Analysis (MFA) was conducted based on means of significant attribute intensities using Time Point as groups to visualize the sensory profiles over time. The MFA compromised space are generated using the "FactoMineR" package, and the score plot and loading plot were generated using the "factoextra" package.

6-4. Results

6-4.1 Physical and Chemical Measures

Overall, the *TDS* before and after dilution, extraction, and titratable acidity increased as brew time increased as shown in Figure 6-2. All coffees were brewed to set times, which corresponded to target timepoints dependent on temperature. The 92°C brews reached higher equilibrium *TDS* before dilution than the 22°C and 4°C brews, with averages of $(3.97 \pm 0.63)\%$, $(3.93 \pm 0.10)\%$, and $(3.52 \pm 0.59)\%$ at the final timepoint, respectively. Consistent with previous studies (Batali et al., 2022), roast level also affected the extraction dynamics, with the light roast being extracted faster and reaching higher *TDS* values than the dark roast at every time point, with this effect being the most pronounced for the 4°C brews. Coffee brews were diluted by a factor of two for sensory evaluations and chemical measurements. Thus, the *TDS* after dilution and calculated extraction yield based on the concentrated *TDS* followed the same trends as the *TDS* before dilution.

The titratable acidity of the coffee samples varied significantly for roast, temperature, and brew time, while the pH only varied significantly with roast and temperature (cf. Figures 6-2D and 6-2E). The light roast coffee had significantly higher titratable acidity and lower pH. Since titratable acidity is correlated with perceived sourness (Batali et al., 2021), our results indicated that the light roast was more sour/acidic than the dark roast regardless of brewing temperature or brew time. The effect of temperature was smaller compared to that of roast; overall, the titratable acidity increased, and pH slightly decreased with brewing temperature. Furthermore, the titratable acidity of coffee increased with brew time, but pH remained stable as brewing proceeded.

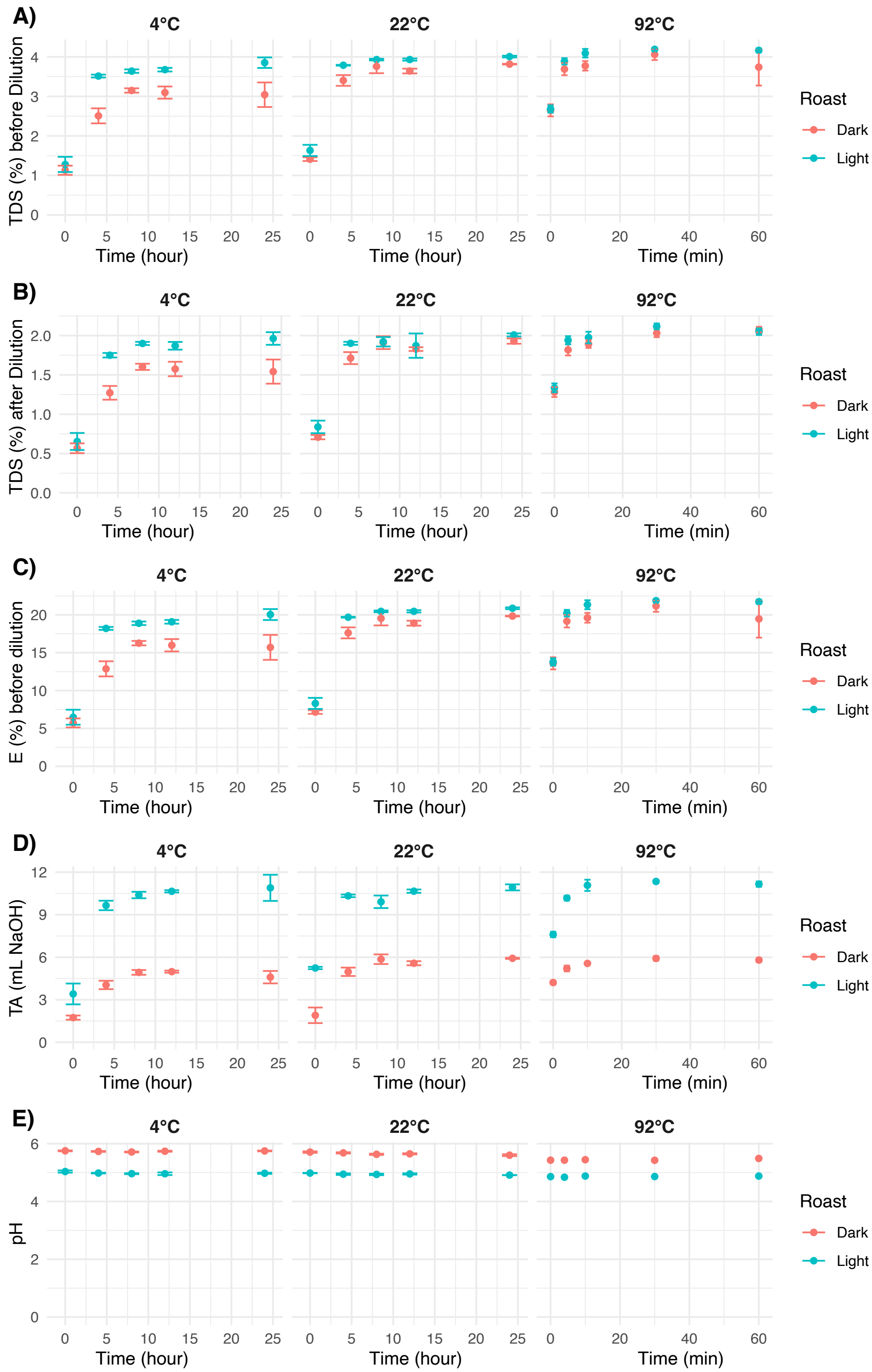


Figure 6-2. Scatter plot of the means and standard deviations of **A)** *TDS* before dilution, **B)** *TDS* after dilution, **C)** Extraction before dilution, **D)** Titratable Acidity, and **E)** pH over time; roast levels are represented with different colors.

6-4.2 Sensory Measures

The three-way MANOVA with two-way interactions across all attributes showed that the main product (coffee samples) effect was significant. In addition, Judge, Rep, and two-way interactions also were significant (p-value < 0.05). Following the significant MANOVA, univariate three-way ANOVAs with two-way interactions for each attribute found that 25 out of the 28 attributes in the scorecard (all attributes except black tea, paper, and herbal) differed significantly among the 30 coffee samples (cf. Supplementary Table 6-S2), indicating a wide range of sensory profiles within this product set. For comparison, the line plots of perceived attribute intensities of all attributes for both roast levels and brewed at three different temperatures over the different time points are shown in Figure 6-3. Within this product set, some attributes intensities varied largely with the experimental factors tested, such as, astringent, bitter, burnt, citrus, cocoa, roasted, rubber, smoky, and sour; while some attributes intensities remained within a smaller range in respect to the change of experimental factors, such as broth, brown spice, brown sugar, cooked green, earthy, floral, savory, whiskey.

Furthermore, the five-way MANOVA examining the effects of experimental factors showed that roast level was the largest driver of differences among the samples, followed by brewing temperature, then brew time, especially the longer brew times as *TDS* plateaued. Fourteen attributes were found to be significant for all three experimental factors - roast, temperature, and time (i.e., bitter, sour, cocoa, berry, citrus, rubber, nutty, roasted, fermented, burnt, smoky, earthy, and brown spices) (cf. Table 6-1). Additionally, fruity, cooked green, and fresh green were significantly different between roasts; sweet, savory, viscous, astringent, and whiskey were significantly different both among temperatures and across times; and brown sugar differed significantly among temperatures. Notably, many of the significant attributes by roast, temperature, or time showed significant two-way interaction(s) among the three experimental factors.

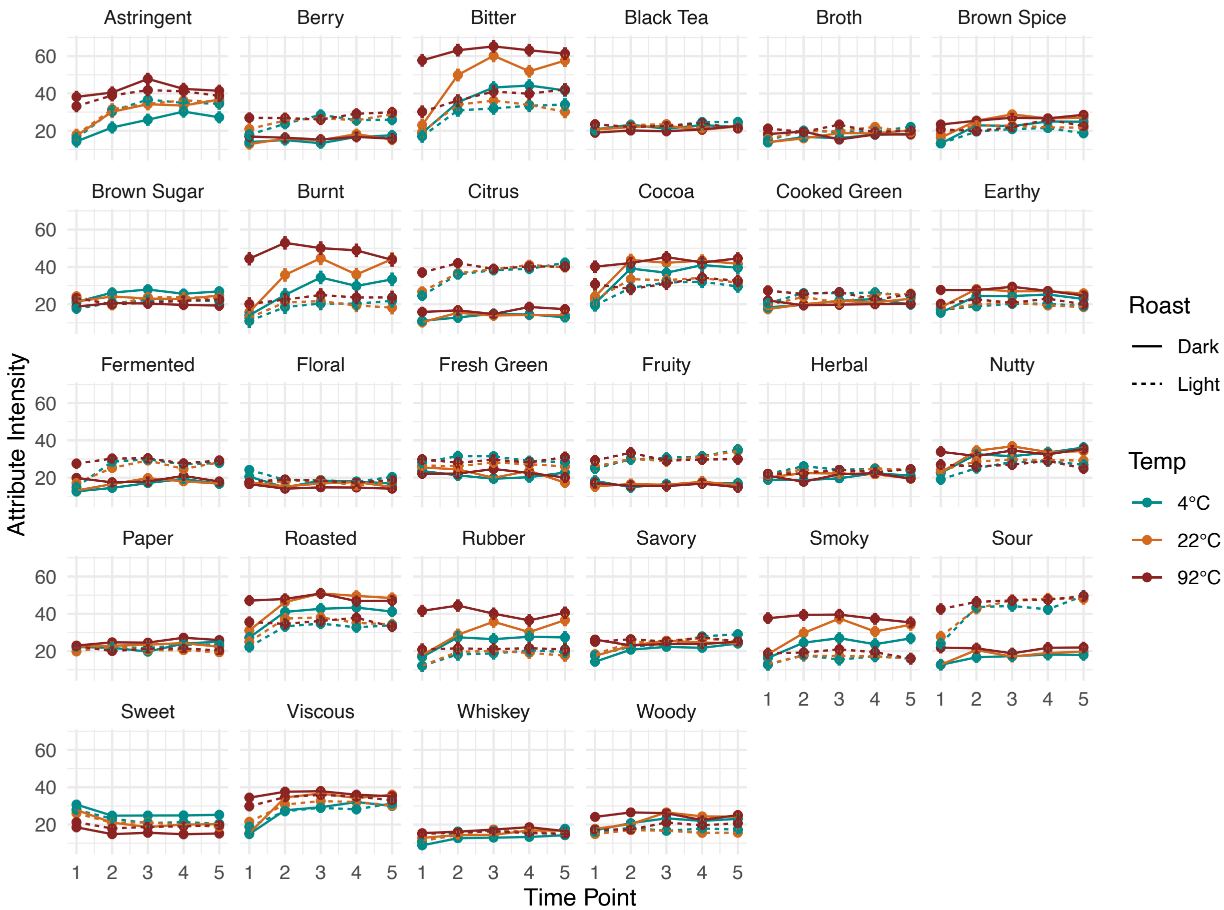


Figure 6-3. Line plots of mean attribute Intensities over time points of light and dark roasts. Time points 1, 2, 3, 4, 5 correspond to 0, 4, 8, 12, 24 hours for 4°C and 22°C brews, and 0, 4, 10, 30, 60 minutes for 92°C brews. Dark roast samples are represented with solid lines, and light roast samples are represented with dashed lines. Different brewing temperatures are represented with different colors, error bars represent the LSD values for each attribute from the 3-way ANOVA with interactions.

Attributes	Roast	Temperature	Time	Roast:Temperature	Roast:Time	Temperature:Time	Roast:Temperature :Time
Bitter	**45.64**	**66.62**	**42.52**	**22.29**	**4.13**	**7.16**	**4.78**
Burnt	**62.15**	**39.92**	**29.94**	**15.26**	**4.80**	**4.45**	**3.01**
Astringent	0.25	**32.69**	**23.68**	**8.69**	0.90	**5.01**	0.95
Smoky	**31.70**	**28.19**	**10.64**	**21.26**	**3.76**	**3.16**	1.22
Rubber	**27.23**	**26.63**	**8.93**	**10.97**	1.89	**5.06**	1.72
Sour	**51.33**	**24.09**	**36.07**	0.31	**4.66**	2.27	1.68
Sweet	0.002	**13.26**	**3.72**	**5.78**	0.21	1.13	0.49
Whiskey	1.38	**9.92**	**8.69**	**4.63**	1.15	1.89	0.49
Citrus	**36.44**	**9.18**	**14.10**	0.03	2.73	1.18	1.86
Earthy	**8.14**	**8.48**	**4.37**	2.53	1.76	1.82	1.37
Fermented	**14.60**	**7.54**	**8.68**	1.72	**9.05**	**3.32**	0.94
Viscous	1.36	**7.46**	**17.89**	**5.57**	**2.61**	**4.74**	**2.89**
Brown Spice	**12.82**	**6.68**	**10.31**	0.28	**2.65**	**2.31**	0.84
Cocoa	**32.30**	**6.35**	**29.64**	2.38	**3.63**	**6.52**	0.73
Woody	**16.36**	**5.83**	**2.93**	2.63	1.66	0.78	**2.47**
Roasted	**29.98**	**5.35**	**13.26**	3.22	1.73	**6.37**	1.10
Berry	**9.64**	**4.56**	**5.68**	1.48	**2.48**	1.25	1.16
Nutty	**11.74**	**3.80**	**15.93**	1.51	2.14	**3.48**	1.04
Savory	2.06	**3.62**	**12.68**	2.53	1.41	**3.50**	0.73
Brown Sugar	3.32	**3.58**	1.85	**6.29**	2.10	1.45	0.44
Paper	1.97	2.30	1.37	**5.57**	1.10	1.09	0.60
Floral	3.26	2.28	2.02	2.07	2.93	1.61	0.64
Fresh Green	**4.98**	1.68	0.85	2.84	1.52	0.96	1.64
Broth	4.07	1.44	2.46	0.32	0.69	1.29	1.48
Cooked Green	**7.12**	1.38	2.32	2.19	0.62	**3.66**	0.81
Black Tea	0.58	0.94	1.44	0.81	0.24	0.85	0.73
Herbal	7.03	0.25	2.05	1.20	1.31	1.00	0.90
Fruity	**18.06**	0.16	2.24	0.12	**3.66**	1.17	0.66

Table 6-1. The F-values of the experimental factors (Roast, Temperature, Time) in the five-way ANOVAs at sensory attributes as response variable. Established significance at 5% are indicated in bold; F-values calculated by pseudo-mixed ANOVA with Judge are in green, F-values calculated by pseudo-mixed ANOVA with Repetition are in blue.

6-4.3 Relation between Sensory and Physical/Chemical Measures

Because the *TDS* and *E* are highly dependent on brew time, the relationship between the attribute intensities and *TDS* were investigated. Correlation analyses revealed that 19 attributes were positively correlated to *TDS* and E, while sweetness was the only attribute negatively correlated with *TDS* and E, and the remaining 8 attributes showed no statistically significant relationship with *TDS* or *E* (cf. Figure 6-4). These findings suggests that most attribute intensities increased with *TDS* as brewing proceeded. Furthermore, correlation analyses between attribute intensities and chemical measurements were also conducted. Sour, berry, fruity, citrus, and fermented had the strongest positive correlations with titratable acidity, and negative correlation with pH, indicating those attributes were highly related to the acid content of the coffees.

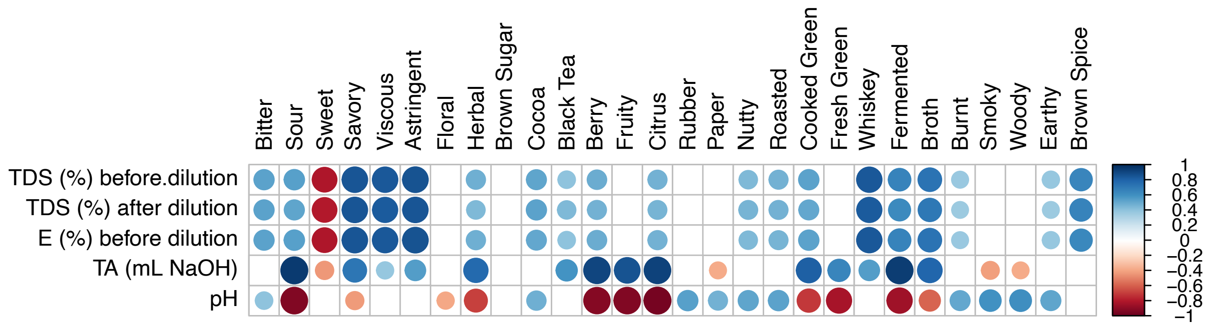


Figure 6-4. Correlations between physical/chemical measurements and attribute intensities. The absolute values of correlation coefficient are reflected by the size of the circles. Significant positive correlations are indicated by blue circles, significant negative correlations are indicated by red circles, and the non-significant correlations at 5% significant level are in blank.

6-4.4 Effects of Roast, Temperature, and Time

The 5-way ANOVA results show that the 17 attributes were significantly different by roast, as the largest driver of difference among the 30 coffee samples (Table 6-1). Roast level had the biggest effects on the following attributes in order of magnitude - burnt, sour, bitter, citrus, cocoa, smoky, roasted, rubber, and fruity, indicated by decreasing F-values (Table 6-1). Overall, dark roast coffee brews had significantly higher bitter, burnt, smoky, roasted, rubber and cocoa intensities, while the light roast coffee brews were significantly more sour, citrus, berry, and fruity (cf. Figure 6-3), which is consistent with prior work (Batali et al., 2022). Notable, fruity was only significant for roast, suggesting that fruity flavor of coffee was dominantly determined by roast level with light roast being significantly fruiter regardless of brewing process tested.

Temperature was the second largest driver of difference of the three experimental factors, with 20 attributes significantly different by temperature from the 5-way ANOVA results. Similarly, bitter, burnt, smoky, rubber, sour; additionally, astringent, sweet, whiskey, citrus and earthy are also important attributes that varied by temperature (cf. Table 6-1). Sweetness significantly increased with decreasing temperature in dark roast, and the sweetness in the 92°C light roast was significantly lower than in the 4 or 22°C brews (cf. Figure 6-5A). In contrast, sour and citrus were significantly higher in the 92°C brews for both roast levels, due to the low perceived flavor intensities in the “rinsed” coffee at 22° and 4 °C (cf. Figures 6-5I and 6-5J). Furthermore, many of the differences by temperature also depended on the roast. For dark roast, bitter, burnt, smoky, rubber, astringent, whiskey, and earthy notes significantly increased with brewing temperature from 4°C, 22°C, to 92°C, while the changes with respect to temperature in light roast were not significant between the 4°C and 22°C brews (cf. Figures 6-5B to 6-5H). These attribute intensities were significantly lower than 92°C brews, except for whiskey, due to the same reason that the “rinsed” coffee at 22°C and 4 °C were lack of flavors.

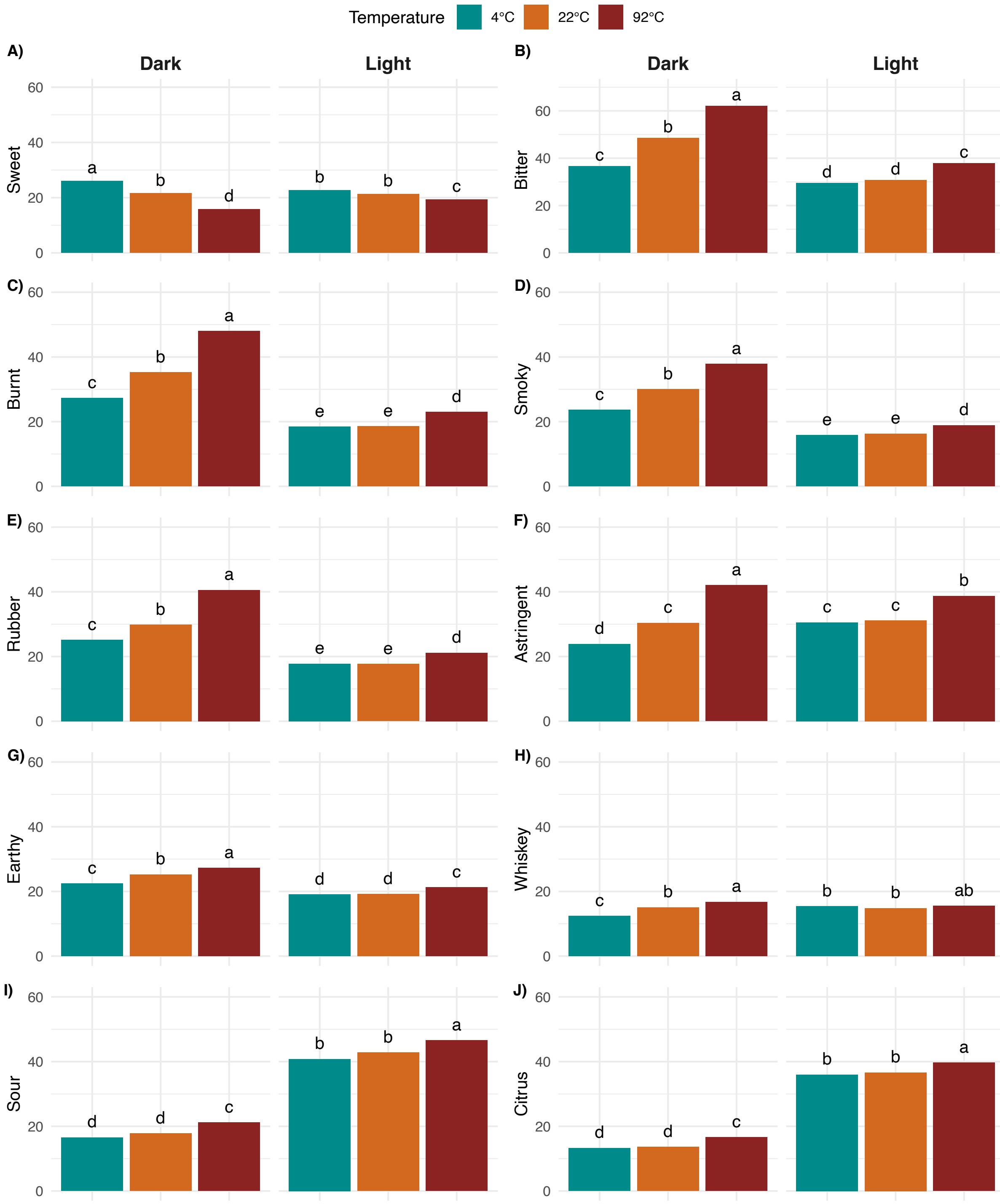


Figure 6-5. Sensory attributes with significant differences by temperature and roast level across all time points, with different letter codes indicating significant difference.

Surprisingly, the effect of time was the smallest within the experimental factors tested. In general the time Point 1 "rinsed" coffee as sweeter, while the other significant attributes were in significantly lower intensities. Interestingly, astringent and viscous, as mouthfeel attributes, were only significant for temperature and time. Regardless of roast level, at 4°C and 22°C, both astringency and viscous mouthfeel generally increased with time (cf. Figure 6-6). Despite the fact the "rinsed" coffee was significantly lower intensity than all the other brews, the fridge and room brews for 8, 12, and 24 hours were significantly more astringent than the 4 hours brew, and the 12- and 24-hours fridge brews were significantly more viscous than the 4 hours brew. At 92°C, the "rinsed" coffee was significantly lower in both viscous mouthfeel and astringency compared to the other timepoints. Furthermore, the effect of time was more pronounced at lower brewing temperature, but it also depended on roast level for specific attributes (cf. Figure 6-7). For example, for dark roast, the changes of bitter and burnt were significant over time point in fridge and room brews, while the changes in hot brews remained relatively stable. Conversely, sour and citrus had more pronounced differences for light roast at lower temperature brews, such that the Light – 4°C – 24hr brew had significantly higher sour and citrus notes compared to the Light – 4°C – 4hr brew.

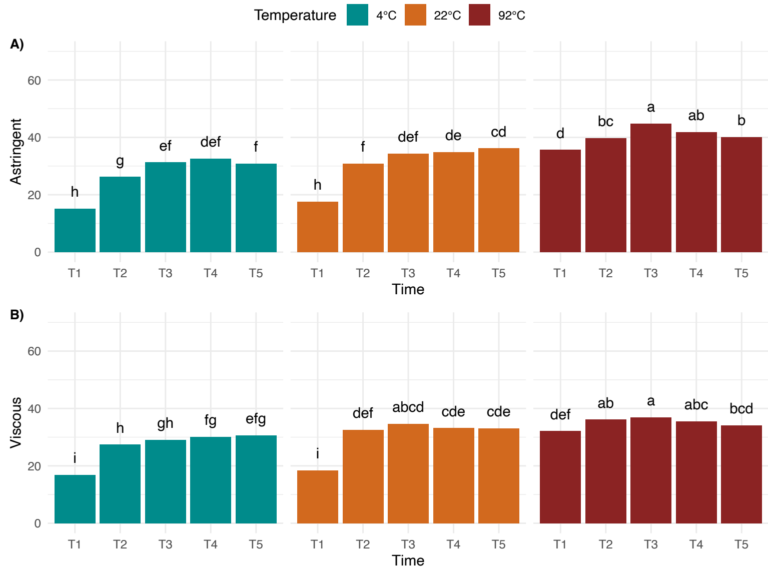


Figure 6-6. Sensory attributes with significant differences by temperature and time point across all roast levels, with different letter codes indicating significant difference.

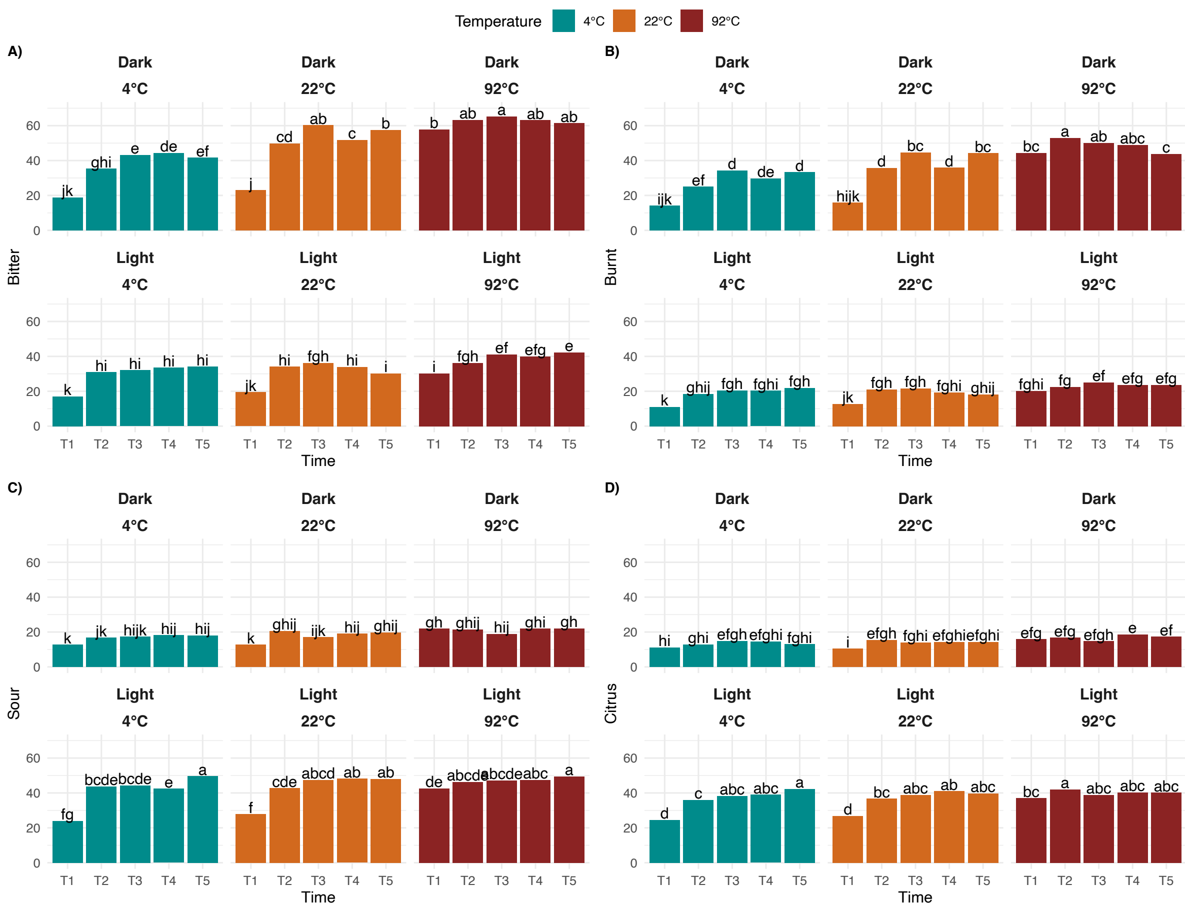


Figure 6-7. Sensory attributes with significant differences by roast level, temperature, and time point, with different letter codes indicating significant difference.

6-4.5 Principal Component Analysis (PCA)

The correlation PCA biplot of the 25 significant attributes on 30 coffee samples is shown in Figure 6-8. The first two dimensions combined explained 84.8% of the total variance, and the third dimension explained another 5.98%. These results accord with the 5-way MANOVA, as the coffee samples were separated the most by roast level. More specifically, attributes that relate dark roast characteristics, for example, burnt, smoky, roasted, rubber, and bitter, are important variables contributed to the first dimension; and other attributes including fermented, savory, broth, sour, are important contributors to the second dimension of the PCA (cf. Supplementary Figure 6-S1). Additionally, the 0-min “rinsed” coffee at 4°C and 22°C were very different from all the other brews with much higher sweet and floral intensities and lack of other flavors.

Furthermore, the PCA further demonstrates that the effect of brewing temperature depended on roast level. For dark roast coffee brews, there was a separation by temperature, such that the 4°C brews were higher in sweet, and floral intensities, 92°C brews were more bitter, burnt, smoky, and astringent, and the 22°C brews were somewhere in between. For light roast coffee, the separation of samples between different temperatures were less clear on the PCA biplot. Similarly, the effect of brew time also depended on brewing temperature. In addition to the 0-min “rinsed” coffee at 4°C and 22°C being unique compared to all the other samples, clearer separations between coffee at lower brewing temperature are shown. More specifically, the dark roast brewed at 4°C exhibited a trend of shorter brews were sweeter and less bitter, roasted, or burnt. However, coffee brews at 92°C, at a given roast level, were very similar to each other.

Interestingly, for light roast, the 92°C “rinsed” coffee (L-92-T1) was also very close to some of the 4°C and 22°C brews, such as samples L-4-T3 and L-4-T4, as shown in the PCA biplot.

Furthermore, the p-values from multivariate pairwise comparisons between the coffee samples, except the "rinsed" coffee at 4 and 22°C, are shown in Table 6-2. The Hotelling's T2 test results revealed that, for light roast coffee, the sensory profiles of these long-time cold brews and short-time hot brews were not significantly different from each other, suggesting that the sensory properties of these coffees were similar (although not necessarily tasted identical). However, this finding is roast dependent, and for dark roast, the short-time hot brews were significantly different from almost all of the long-time cold brews.

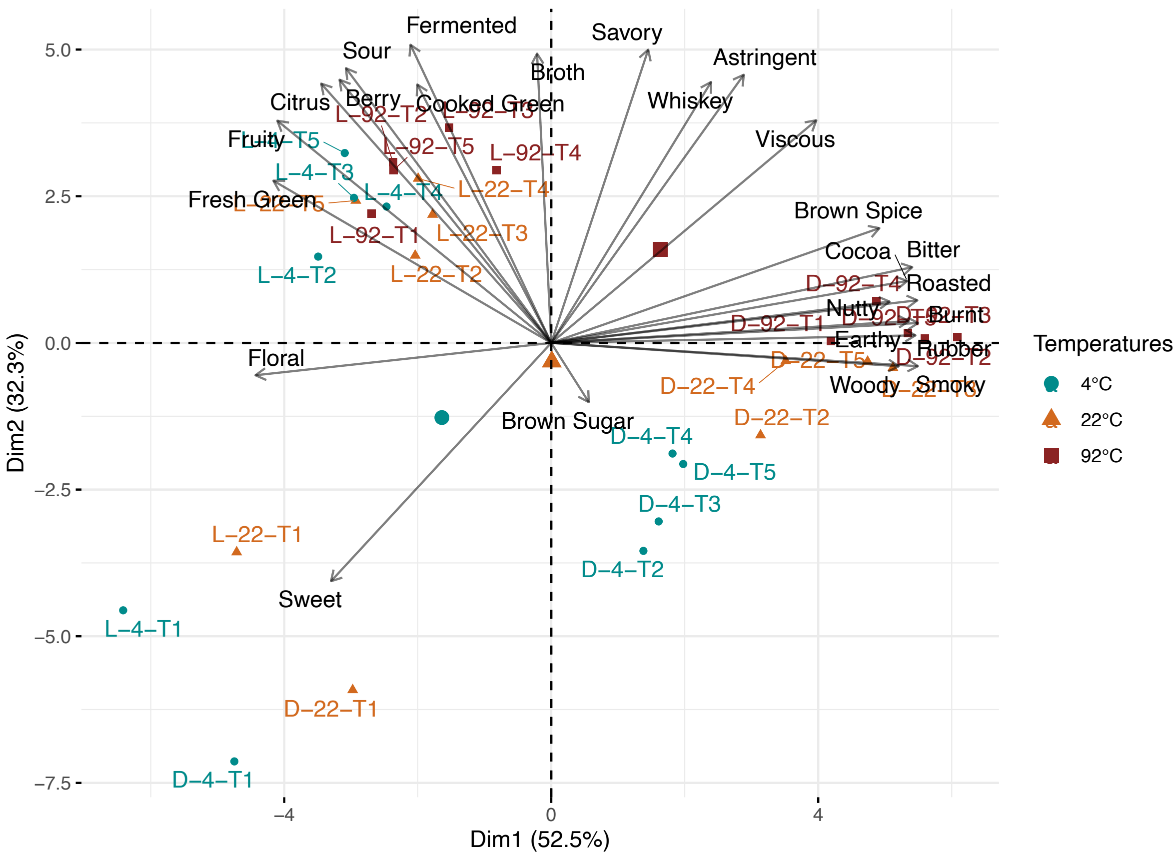


Figure 6-8. Principal component analysis biplot of coffee samples and significant sensory attributes from 3-way ANOVA. Different brewing temperatures are indicated by different colors. Nomenclature of the coffee samples are represented by: Roast (L: light roast / D: dark roast) – Temperature (4/22/92°C) – Time Point (T1/T2/T3/T4/T5). Time points T1, T2, T3, T4, T5 corresponds to 0, 4, 8, 12, 24 hours in 4°C and 22°C brews, and 0, 4, 10, 30, 60 minutes in 92°C brews. See Supplementary Figure 1 for important contributors to the first two PCs.

A)

	Light-4C-T2	Light-4C-T3	Light-4C-T4	Light-4C-T5	Light-22C-T2	Light-22C-T3	Light-22C-T4	Light-22C-T5	Light-92C-T1	Light-92C-T2	Light-92C-T3	Light-92C-T4	Light-92C-T5
Light-4C-T2	1.0E+00	3.4E-01	4.5E-01	3.2E-03	3.6E-01	9.7E-03	4.7E-02	5.0E-02	8.0E-01	9.0E-04	1.5E-04	7.3E-05	7.0E-05
Light-4C-T3	3.4E-01	1.0E+00	5.3E-01	8.8E-02	6.9E-01	1.7E-01	3.5E-01	4.8E-01	5.0E-01	2.5E-02	2.2E-03	1.2E-03	1.2E-03
Light-4C-T4	4.5E-01	5.3E-01	1.0E+00	2.0E-03	9.8E-01	5.0E-02	6.9E-02	2.2E-02	7.7E-01	2.8E-03	3.1E-04	2.8E-04	5.0E-04
Light-4C-T5	3.2E-03	8.8E-02	2.0E-03	1.0E+00	2.9E-02	3.4E-01	7.6E-01	4.6E-01	9.1E-04	2.1E-01	1.3E-02	1.3E-03	2.6E-03
Light-22C-T2	3.6E-01	6.9E-01	9.8E-01	2.9E-02	1.0E+00	1.2E-01	1.6E-01	1.5E-01	6.8E-01	1.7E-02	1.6E-03	1.3E-03	1.5E-03
Light-22C-T3	9.7E-03	1.7E-01	5.0E-02	3.4E-01	1.2E-01	1.0E+00	7.7E-01	4.3E-01	1.2E-02	6.6E-01	6.2E-02	3.1E-02	4.8E-02
Light-22C-T4	4.7E-02	3.5E-01	6.9E-02	7.6E-01	1.6E-01	7.7E-01	1.0E+00	7.3E-01	5.7E-02	6.1E-01	5.0E-02	1.1E-02	2.6E-02
Light-22C-T5	5.0E-02	4.8E-01	2.2E-02	4.6E-01	1.5E-01	4.3E-01	7.3E-01	1.0E+00	2.6E-02	1.8E-01	1.4E-02	5.4E-03	8.8E-03
Light-92C-T1	8.0E-01	5.0E-01	7.7E-01	9.1E-04	6.8E-01	1.2E-02	5.7E-02	2.6E-02	1.0E+00	4.7E-04	7.8E-05	4.3E-05	6.8E-05
Light-92C-T2	9.0E-04	2.5E-02	2.8E-03	2.1E-01	1.7E-02	6.6E-01	6.1E-01	1.8E-01	4.7E-04	1.0E+00	1.4E-01	4.3E-02	1.0E-01
Light-92C-T3	1.5E-04	2.2E-03	3.1E-04	1.3E-02	1.6E-03	6.2E-02	5.0E-02	1.4E-02	7.8E-05	1.4E-01	1.0E+00	7.4E-01	9.3E-01
Light-92C-T4	7.3E-05	1.2E-03	2.8E-04	1.3E-03	1.3E-03	3.1E-02	1.1E-02	5.4E-03	4.3E-05	4.3E-02	7.4E-01	1.0E+00	6.1E-01
Light-92C-T5	7.0E-05	1.2E-03	5.0E-04	2.6E-03	1.5E-03	4.8E-02	2.6E-02	8.8E-03	6.8E-05	1.0E-01	9.3E-01	6.1E-01	1.0E+00

B)

	Dark-4C-T2	Dark-4C-T3	Dark-4C-T4	Dark-4C-T5	Dark-22C-T2	Dark-22C-T3	Dark-22C-T4	Dark-22C-T5	Dark-92C-T1	Dark-92C-T2	Dark-92C-T3	Dark-92C-T4	Dark-92C-T5
Dark-4C-T2	1.0E+00	1.2E-01	1.2E-01	2.9E-01	7.1E-03	2.2E-04	5.7E-04	1.2E-04	1.6E-05	4.5E-07	1.3E-06	4.7E-07	4.7E-05
Dark-4C-T3	1.2E-01	1.0E+00	7.0E-01	6.8E-01	3.1E-03	3.1E-03	6.4E-03	1.0E-03	1.9E-05	2.9E-07	3.9E-06	2.2E-07	2.4E-05
Dark-4C-T4	1.2E-01	7.0E-01	1.0E+00	7.7E-01	3.4E-02	2.1E-03	4.7E-03	5.6E-04	5.0E-05	5.8E-07	1.7E-06	8.3E-07	1.9E-04
Dark-4C-T5	2.9E-01	6.8E-01	7.7E-01	1.0E+00	1.1E-01	1.3E-03	4.1E-03	7.6E-04	5.3E-04	9.9E-06	4.1E-06	1.9E-05	1.1E-03
Dark-22C-T2	7.1E-03	3.1E-03	3.4E-02	1.1E-01	1.0E+00	2.4E-03	1.9E-02	4.8E-03	1.0E-02	7.6E-05	2.1E-05	1.8E-04	1.7E-02
Dark-22C-T3	2.2E-04	3.1E-03	2.1E-03	1.3E-03	2.4E-03	1.0E+00	1.8E-01	4.1E-01	4.5E-02	2.0E-03	1.9E-02	3.4E-04	5.7E-03
Dark-22C-T4	5.7E-04	6.4E-03	4.7E-03	4.1E-03	1.9E-02	1.8E-01	1.0E+00	4.9E-01	3.6E-02	5.0E-04	2.0E-03	3.7E-04	1.9E-02
Dark-22C-T5	1.2E-04	1.0E-03	5.6E-04	7.6E-04	4.8E-03	4.1E-01	4.9E-01	1.0E+00	1.7E-01	5.3E-03	2.6E-02	2.0E-03	4.7E-02
Dark-92C-T1	1.6E-05	1.9E-05	5.0E-05	5.3E-04	1.0E-02	4.5E-02	3.6E-02	1.7E-01	1.0E+00	2.7E-01	3.7E-01	1.3E-01	6.7E-01
Dark-92C-T2	4.5E-07	2.9E-07	5.8E-07	9.9E-06	7.6E-05	2.0E-03	5.0E-04	5.3E-03	2.7E-01	1.0E+00	5.3E-01	2.8E-01	7.3E-01
Dark-92C-T3	1.3E-06	3.9E-06	1.7E-06	4.1E-06	2.1E-05	1.9E-02	2.0E-03	2.6E-02	3.7E-01	5.3E-01	1.0E+00	2.6E-02	2.5E-01
Dark-92C-T4	4.7E-07	2.2E-07	8.3E-07	1.9E-05	1.8E-04	3.4E-04	3.7E-04	2.0E-03	1.3E-01	2.8E-01	2.6E-02	1.0E+00	5.7E-01
Dark-92C-T5	4.7E-05	2.4E-05	1.9E-04	1.1E-03	1.7E-02	5.7E-03	1.9E-02	4.7E-02	6.7E-01	7.3E-01	2.5E-01	5.7E-01	1.0E+00

Table 6-2. p-values of the Hotelling's T2 tests for pairwise comparison of sensory profiles between A) light roast and B) dark roast coffee samples. "t=0" coffees brewed at 4°C and 22°C were excluded from the analysis. Significance at 5% is indicated in light red.

6-4.6 Multiple Factor Analysis (MFA)

The result of the MFA using time points as a reflection of extraction stages as groups is shown in Figure 6-9. The first two dimensions accounted for 85.9% of the total variance, and the third dimension explained another 5.7%. Again, samples were separated primarily by roast level, then by brewing temperature, with the light roasts on the left and dark roast on the right of the first dimension (cf. Figure 6-9A). The partial axes plot also revealed that the differences that varied by temperature also depended on the roast level. More specifically, light roast coffees brewed at 4°C and 22°C were closer to each other compared to the 4°C and 22°C brews from the dark roast, indicating that room and fridge brews using light roast coffee were more similar to each other compared to those brewed using the dark roast (cf. Figure 6-9A). The MFA further demonstrates that light roast coffee samples across brew temperature and brew time are more similar to each other compared to the dark roast coffee samples, since they are positioned closer to each other with shorter partial axes. Thus, it is consistent with the multivariate pairwise comparison results that the sensory profiles of short hot brews and long cold brews were more similar in light roast coffee. Furthermore, the coffee samples from Time Point 1 is again the most different from the other Time Points, while the coffee brewed after the "rinsed" stage are much closer to each other (cf. Figure 6-9B). Moreover, the correlation circles of variables at different time points also showed that the sensory profiles of this product set did not alter very much after Time Point 1 (cf. Figure 6-9C), indicating the longer brew times had a much smaller effect on the sensory profiles of full immersion brewed coffee compared to roast level and brewing temperature.

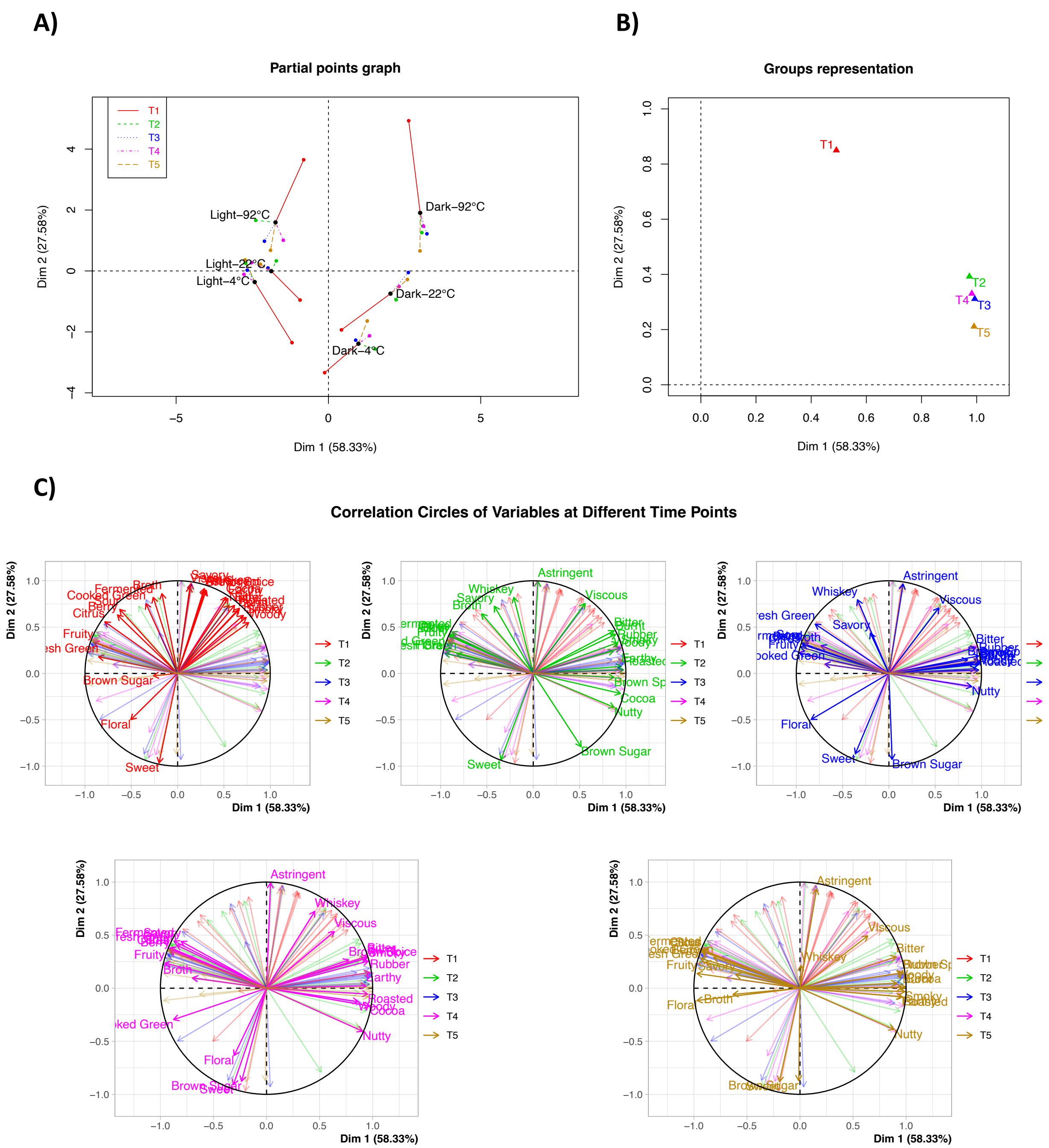


Figure 6-9. A) Individual factor map with partial axes correlation plot, **B)** group representation, and **C)** correlation circles by group from MFA using time points (T1, T2, T3, T4, T5) as groups.

6-5. Discussion

6-5.1 The Effect of Brew Time

Our analyses consistently found that brew time was the least substantial driver of sensory differences among the full immersion brewed coffee samples compared to roast level and temperature, at least for the longer brew times examined here. Coffees from Time Point 1 (the "rinsed concentration") were clearly different from the rest of the coffees regardless of roast or brewing temperature; yet, few statistically significant changes were observed in the sensory profiles of coffees brewed beyond Time Points 3 as *TDS* plateaued. Another reason why brew time had such a small effect possibly is that Time Point corresponded to each extraction stage as a factor were used instead of the actual continuous brew time as a parameter. Because the variance within treatment is larger due to the natural difference in *TDS* within the same Time Point at different brewing temperature (cf. Supplementary Figure 6-S2), it is harder to find differences compared to the variance between treatments. Thus, there is more control over roast level and brewing temperature, but comparatively less control over the final *TDS* corresponding to different brew times at different brewing temperatures due to the natural difference in extraction dynamics of full immersion brews (as shown in Chapters 3 through 5).

Similarly, a previous fractionation study of the flavor profiles of drip brew coffee over time had also found strong correlations between attribute intensities and *TDS*, which was naturally imposed by brew time (Batali et al., 2020a). In the present study, we found that bitterness, sourness and astringency were positively correlated with *TDS*, whereas sweetness was negatively correlated to *TDS*. It is important to note that, the coffee samples evaluated in full immersion brews were at their accumulative *TDS* from $t = 0$ brewed up to a certain time point; in contrast, coffee samples evaluated in the drip brew study at their instantaneous *TDS*, which corresponds to a fraction of a "whole brew", in which each fraction were at 30-second increments of the brewing period. This suggests that *TDS*, rather than the actual brew time, acts as the factor driving flavor in both drip brew and full immersion brews. Interestingly, sweet and floral attributes were perceived with higher intensity towards the end of the drip brew, while sweetness was perceived as more intense at the beginning of full immersion brews, in both cases due to the lower *TDS* levels. Here, the perception of sweetness is more related to the impression of sweetness and the absence or low level of other flavors such as bitterness and acidity rather than actual perceived sweetness (Batali et al., 2020b, 2020a; Guinard et al., 2023). Additionally, the lack of a significant correlation between floral and *TDS* in this study might be due to the specific beans used, as floral was not a significant attribute within the coffee samples set we tested, and the effect of coffee producing origin was found to be the second most influential factor in the variations among full immersion brewed coffee (Batali et al., 2020b). This observation suggests that the floral characteristics of the South American blend used in this study might not have been pronounced, and other coffees may be impacted differently by brew time.

6-5.2 Short-time Hot Chilled Brews vs. Long-time Cold brews

An interesting finding is that the sensory profiles of certain short-time hot brews, especially the 92°C "rinsed" coffee, were similar to those of long-time cold brews at 4°C and 22°C for the light roast coffee we used, indicating an overlap in sensory perception between short-time hot brew and long-time cold brew using full immersion brewing technique. Yet, the extent of this overlap remains unclear and appears to be dependent on the roast level of the coffee, as this overlap was much larger in the particular light roast coffee we used in this study. In contrast, the dark roast yielded a statistically significant difference between the short hot brew and long cold brew. To further explore this finding rigorously, discrimination testing will be needed to compare coffee samples brewed from long-time-cold-temperature and short-time-hot-temperature from a wider range of pre-brewing conditions including origins, processing methods, storage conditions, and roast levels.

Furthermore, other coffee brewing and coffee serving parameters also contribute to this overlap. In our experimental approach, we brewed the coffee concentrate and then diluted it by a factor of 2 the day prior to sensory evaluation, then the coffee beverages were chilled in the refrigerator before serving. In this manner we attempted to minimize the effect of varied serving temperature on sensory perceptions, by serving all coffee samples at a controlled cold temperature. As a consequence of this approach, however, another potential confounding factor is that the overnight storage time might affect the chemical composition and sensory profiles of coffee while is stored at refrigerated temperature (Pérez-Martínez et al., 2008). More detailed chemical analysis is necessary to test this hypothesis.

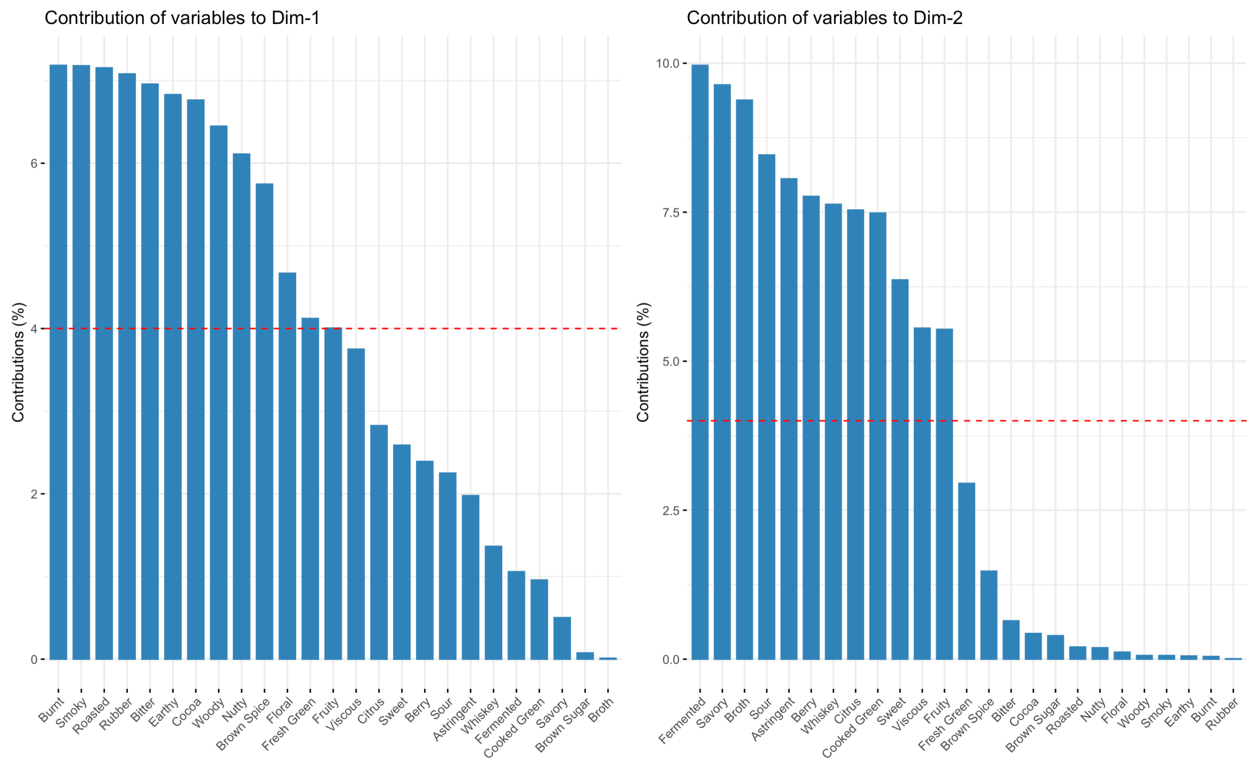
6-5.3 Practical Implications

The overarching finding from our sensory analysis is that roast was the main driver of the overall flavor profile of full immersion brewed coffee, while temperature and time provided tools to optimize attribute intensities for the flavor profile of the roasted coffee beans we used. For instance, fruity flavor, as an important driver of consumer liking (Batali et al., 2020b; Cotter et al., 2021; Frost et al., 2020; Guinard et al., 2023), was only significant by roast level, suggesting that darker roasts may hinder the expression of fruitiness regardless of brewing temperature or brew time. Previous sensory analysis of full immersion brew that examined the flavor profile of full immersion brews at fixed *TDS* found that the difference within the coffee sample is driven by roast level, origin, and then by temperature (Batali et al., 2020b). Thus, when aiming to achieve specific sensory properties of coffee using full immersion brewing technique, it is crucial for practitioners to prioritize designing the roast of the coffee beans, followed by the temperature, and lastly, the longer brew times, especially after Time Point 3 as the *TDS* approaches equilibrium. When brewing light roast coffee, it is worth considering the possibility of achieving similar sensory profiles of long-time cold brews using short-time chilled hot brews through controlled preparation method. Although similar flavor profiles can be obtained in a shorter time, the energy required for brewing water and chilling the coffee should be considered. From efficiency improvement aspects, a noteworthy implication is the potential for shorter brew times in crafting cold brew than conventionally assumed. The current general practice of cold brew falls between 12 to 24 hours (Cordoba et al., 2019; Fuller and Rao, 2017; Portela et al., 2021; Toddy, 2020). We observed very few statistically significant changes in the sensory profiles after Time Point 3 (8 hours at 4°C and 22°C), suggesting that the industry can increase efficiency in full immersion styled cold brew coffee by reducing brew time without changing any other brewing conditions.

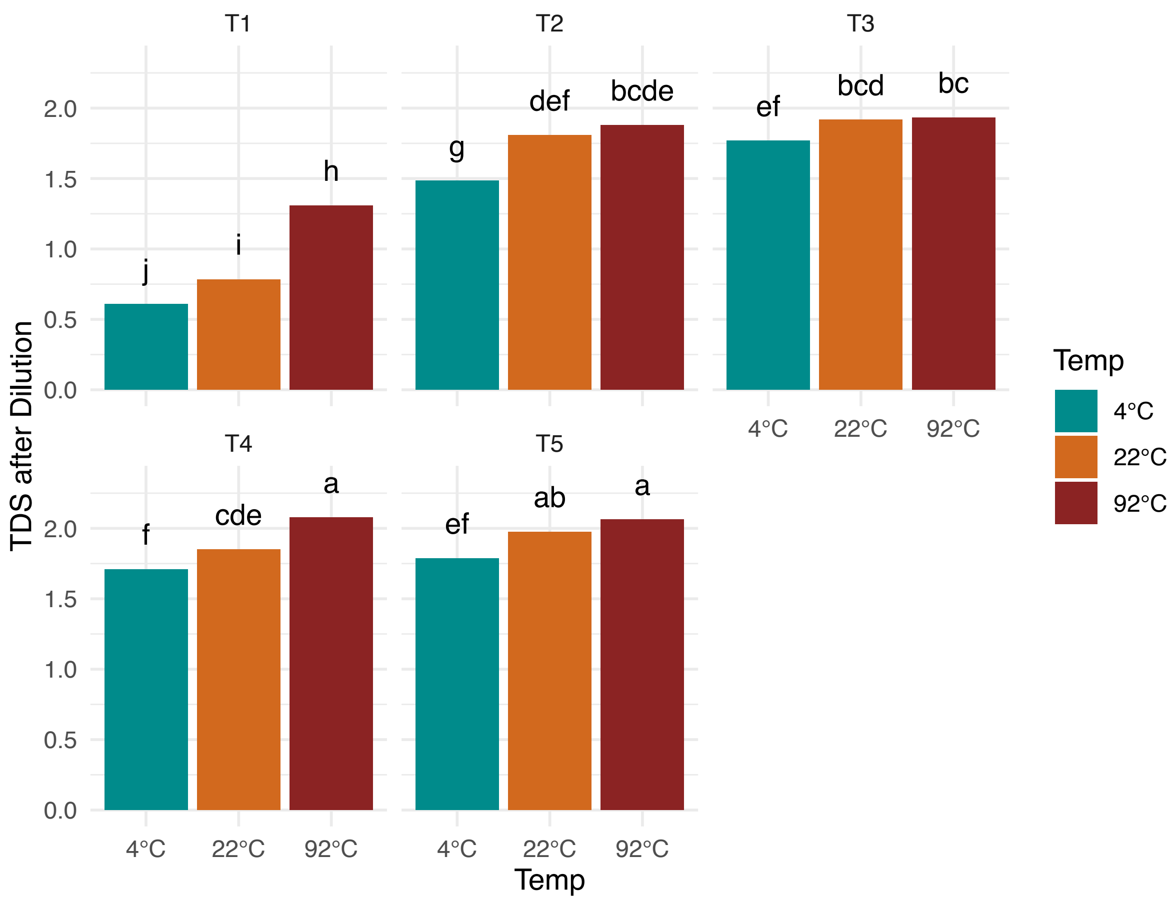
6-6. Conclusions

Our study demonstrated the significant impact of roast level, temperature, and brew time on the sensory quality of full immersion brews. A wide range of flavor profiles were achieved from a single source green coffee blend through combination of these factors, with roast level as the biggest driver of flavor, followed by temperature, then by the longer brew time points as *TDS* plateaued. Furthermore, perceived sweetness was negatively correlated with *TDS*, while 19 other attributes had a significant positive correlation with *TDS*. Interestingly, certain short-time hot brews, especially the 92°C "rinsed" coffee, had similar sensory profiles to those of long-time cold brews at 4°C and 22°C for light roast, although this similarity may depend on roast level and characteristics of the coffee beans used. These findings provide valuable understandings of the effects of coffee preparation factors on extraction and sensory profiles of full immersion coffee over time, and bring new practical insights into the control of sensory quality of full immersion brews for the coffee industry.

Supplementary Materials



Supplementary Figure 6-S1. Bar plots of the important contributors to PC 1 and PC 2 in the PCA. This dashed line corresponds to the expected value if the contributions were uniform.



Supplementary Figure 6-S2. *TDS* after dilution by temperature and time point across roast levels, with different letter codes indicating significant difference.

Attributes	Reference Standards
Bitter	Basic taste of bitter (0.1% caffeine solution in water)
Sour	Basic taste of sour (1.25% citric acid solution in water)
Sweet	Basic taste of sweet (2% sugar solution in water)
Savory	Basic taste of umami (1% MSG solution in water)
Viscous	Thick-It Clear Advantage Thickened Water
Astringent	Mouth-drying, puckering feeling (2% alum solution in water)
Floral	Dry Celestial Seasonings chamomile lavender tea
Herbal	Dried parsley
Brown Sugar	C&H Pure Cane Sugar, Golden Brown
Cocoa	Hershey's Unsweetened Cocoa Powder
Black Tea	Brewed Lipton black tea
Berry	mixed berries (blackberry, strawberry, raspberry, blueberry)
Fruity	Signature Select mixed fruit (White Grape Juice From Concentrate, Pineapple, Peaches, Pears, Cherry)
Citrus	Fresh sliced lemon and orange
Rubber	Cut pieces of bicycle inner tube
Paper	damp cardboard
Nutty	Justin’s almond butter
Roasted	Roasted barley
Cooked Green	Green Giant cut green beans
Fresh Green	Sliced green bell pepper and cucumber
Whiskey	Jack Daniels Tennessee Whiskey
Fermented	Guinness dark beer
Broth	Better than Bouillon roasted vegetable concentrate
Burnt	French Roast coffee
Smoky	Wright's Liquid Smoke
Woody	Twigs and Cedar balls
Earthy	Damp Miracle-Gro Potting Soil
Brown Spice	Equal parts cinnamon, nutmeg, clove, and allspice

Supplementary Table 6-S1. Reference standards used for the sensory attributes chosen by the panelists.

Attribute	ANOVA		Pseudo-mixed ANOVA using Product*Judge		Pseudo-mixed ANOVA using Product*Rep	
	F value	p-value	F value	p-value	F value	p-value
Bitter	48.1477	< 2.2e-16 ***	**28.89**	**<2e-16 *** **	34.82	<2e-16 ***
Sour	60.9065	< 2.2e-16 ***	**32.97**	**<2e-16 *** **	28.79	<2e-16 ***
Sweet	7.3594	< 2.2e-16 ***	**3.267**	**8.92e-08 *** **	N/A	N/A
Savory	5.2356	< 2.2e-16 ***	**3.816**	**8.44e-10 *** **	N/A	N/A
Viscous	16.1833	< 2.2e-16 ***	**7.246**	**<2e-16 *** **	N/A	N/A
Astringent	19.7316	< 2.2e-16 ***	**10.19**	**<2e-16 *** **	N/A	N/A
Floral	2.5905	1.211e-05 ***	**2.075**	**0.00115 ** **	N/A	N/A
Herbal	2.1729	0.0003898 ***	N/A	N/A	1.486	0.0995
Brown Sugar	2.4186	5.234e-05 ***	**2.093**	**0.00101 ** **	N/A	N/A
Cocoa	14.0112	< 2.2e-16 ***	**10.97**	**<2e-16 *** **	N/A	N/A
Black Tea	0.9153	0.5958639	-	-	-	-
Berry	11.6807	< 2.2e-16 ***	**6.248**	**<2e-16 *** **	N/A	N/A
Fruity	18.5152	<2e-16 ***	**8.967**	**<2e-16 *** **	N/A	N/A
Citrus	59.4370	< 2.2e-16 ***	**24.14**	**<2e-16 *** **		
Rubber	21.5944	< 2.2e-16 ***	**13.69**	**<2e-16 *** **	N/A	N/A
Paper	1.9136	0.002835 **	1.123	0.305	N/A	N/A
Nutty	7.2648	< 2.2e-16 ***	**5.203**	**5.71e-15 *** **	N/A	N/A
Roasted	20.4556	< 2.2e-16 ***	**9.891**	**<2e-16 *** **	N/A	N/A
Cooked Green	3.1679	6.818e-08 ***	**2.606**	**2.02e-05 *** **	N/A	N/A
Fresh Green	5.4657	< 2.2e-16 ***	**2.494**	**4.87e-05 *** **	N/A	N/A
Whiskey	3.1173	1.088e-07 ***	**2.12**	**0.000833 *** **	N/A	N/A
Fermented	15.4128	< 2.2e-16 ***	**8.249**	**<2e-16 *** **	N/A	N/A
Broth	**2.5555**	**1.637e-05 *** **	N/A	N/A	N/A	N/A
Burnt	31.0645	< 2.2e-16 ***	**24.47**	**<2e-16 *** **	N/A	N/A
Smoky	22.8506	< 2.2e-16 ***	**14.47**	**<2e-16 *** **	N/A	N/A
Woody	7.2134	< 2.2e-16 ***	**4.522**	**1.96e-12 *** **	N/A	N/A
Earthy	6.4763	< 2.2e-16 ***	**4.486**	**2.67e-12 *** **	N/A	N/A
Brown Spice	7.6666	< 2.2e-16 ***	**5.168**	**7.69e-15 *** **	N/A	N/A

Supplementary Table 6-S2. F value and p-value of main product effect (Coffee) in three different ANOVAs for each attribute. Statistical significance at (p<0.05) is denoted by *. Attributes with significant main product effect are indicated in bold.

Chapter 7. Conclusions and future work

7-1. Summary of key findings

In this dissertation, we have addressed many practical questions that are of interest to the coffee industry. These questions are fundamental but crucial in the control of extraction dynamics and the pursuit of desired sensory quality of full immersion brewed coffee. In the first stage of study (Chapter 2), we demonstrated that the equilibrium *TDS* and *E* of full immersion brewed coffee are well-captured using a pseudo-equilibrium desorption model, with a single, species-averaged equilibrium constant K. Experimental data showed that the equilibrium *TDS* is inversely proportional to R_{brew}, and the equilibrium extraction yield is independent over a wide range of R_{brew}. Under the major effect of R_{brew}, K is insensitive to grind size, roast level, and hot brewing temperature over the range 80-99°C. In addition, the oven-drying measured extraction underestimates of the true value at equilibrium, due to the retained liquid within the spent moist grounds. The practical implication from this study is full immersion brewing offers precise control over the *TDS* at equilibrium but little control over E.

In the second stage of the study (Chapters 3 and 4), we showed that the dynamic *TDS* and extraction of full immersion brews over a wide range of coffee preparation parameters, including origin, roast level, brewing temperature, and brew ratio, are well characterized using an updated and extended diffusion-limited mass transfer model with the three key parameters C_{eq}, C_0, and k. We validated this model with an extensive set of experimental data, comprising 3,420 *TDS* measurements. Brewing temperature most strongly impacted the extraction dynamics as expected; most interestingly, roast level was also found to significantly affect the extraction rate, in which the darker roasts extracted slower than lighter roasts, while the effect of origin with different post-harvest processing methods was minimal. In addition, the effective mass transfer coefficient k of the agitated brews, the equilibrium concentration C_{eq} and the “rinse” ratio C_0/C_{eq} of all brews increased with decreasing coffee grounds particle size. Our results further validated that the effective extraction kinetics of coffee solubles in full immersion brews is dominated by internal diffusion through the bean particles, in which k is insensitive to agitation rate. These systematic brewing experiments provide a means of predicting how extraction dynamics respond to key coffee preparation factors and brewing parameters, and offer actionable tools in controlling the *TDS* and *E* of full immersion brews to yield desired brew characteristics to coffee practitioners.

In the third stage (Chapter 5), our experimental work provided one of the first investigations into the role of coffee grounds sedimentation on the concentration profile in a full immersion brew. Our results indicated that ostensibly quiescent full immersion brewed coffee is a highly heterogeneous mixture, in which the *TDS* of liquid coffee differs depending on both time and the specific position within the brew. We observed that the magnitude of the concentration gradient varied over time as the brewing and sedimentation proceed, in which darker roasts sediments slower than light roasts. The practical implications of these findings are 1) the sampling position from the brew matters, and 2) sensory evaluations obtained via the traditional “cupping” method used widely in the coffee industry might be confounded by differences in *TDS* for different roast levels.

In the last stage (Chapter 6), we utilized the understandings of extraction dynamics from the diffusion-limited mass transfer model in combination with sensory descriptive analysis to compare the sensory profiles of full immersion brews over time. We demonstrated that a single source green coffee blend can produce a wide range of complex sensory profiles using different combinations of roast level, temperature, and brew time. Roast level was the biggest driver of differences, followed by temperature, then brew time point corresponding to target extraction stages of full immersion coffee extraction dynamics, especially the longer brew times as *TDS* plateaued. At a given brewing temperature, few statistically significant changes in flavor profiles were observed after equilibrium *TDS* was reached, suggesting potential to increase efficiency by reducing brew time beyond equilibrium. Furthermore, perceived sweetness was found to be negatively correlated with *TDS*, while 19 other attributes had a significant positive correlation with *TDS*. Interestingly, certain short-time hot brews, especially the 92°C "rinsed" coffee, had similar sensory profiles to those of long-time cold brews at 4°C and 22°C under controlled preparation when served at consistent temperature. These findings provide valuable understandings of the effects of coffee preparation factors on the sensory profiles of full immersion coffee over time and bring new practical insights to the industry in the achieving desirable sensory properties using full immersion brewing technique.

Taken together, by integrating food engineering and sensory analysis following a sensory-driven engineering approach, our findings provide valuable insight on the extraction dynamics and sensory quality of full immersion brewed coffee. This series of systematic brewing experiments and sensory analysis adds to expanding field of coffee brewing research and advances the knowledge for continuous improvement in the coffee industry.

7-2. Suggestions for future work and boarder implications

The results presented here highlight several aspects that warrant deeper investigation in future research endeavors. From the extraction dynamics studies, our experimental result indicates that the "rinse" concentration C_0 depends sensitively on temperature and grind size; however, the precise composition of the soluble compounds within the initial "rinsed" extraction remain to be elucidated. Further research is needed to understand the extraction happening in "rinse phase" where rapid dissolution of soluble substances take place.

Another very interesting topic for further exploration is what makes darker roast extract more slowly. We tried to answer this question in Chapter 5 through investigation of coffee grounds sedimentation in quiescent brews; however, brews with different roast levels can also be experimented with agitation to compare the extraction rates under elimination of the sedimentation effect. Furthermore, the composition of soluble coffee compounds is extremely complex, and coffee roasting contributes largely to the reaction and formation of these flavor compounds, resulting in different composition of extractable coffee solubles at different roast levels (Rostagno et al., 2015; Rufián-Henares and Pastoriza, 2015; Sunarharum et al., 2014; Tian et al., 2018; Wei and Tanokura, 2015; Yeager et al., 2021). As one of the major components of coffee beverage, the amount of melanoidins increases with the severity of roasting (Bekedam et al., 2008; Borrelli et al., 2002; Rufián-Henares and Pastoriza, 2015; Wei and Tanokura, 2015). We hypothesize that the slower extraction rate and lower diffusivity in darker roast is due to the accumulation of high molecular weight melanoidins as roasting proceeds. Analytical chemistry approaches coupled with an extraction dynamics study are needed to analyze the composition of coffee soluble over time to understand the roles of solubility or diffusivity of different molecules and how they contribute to the overall extraction process.

From the sedimentation study, our data suggests that difference in sedimentation speed is mainly due to the difference in density at a fixed particle size. The effect of particle size is well worth investigating as a next step to systematically evaluate the application of Stoke's Law in the context of coffee grounds sedimentation in full immersion brewing. More importantly, the release of CO_2 off-gassing during brewing also affects the sedimentation as it contributes to the buoyancy of the top layer of coffee grounds. Because of the higher residual CO_2 content in darker roast coffee grounds (Smrke et al., 2018; Wang and Lim, 2014), we hypothesize that the slower sedimentation rate in dark roast could possibly due to the release of more CO_2 during brewing, along with the changing density and porosity in coffee grounds. Overall, the coffee off-gassing phenomenon during brewing remains underexplored. Future studies would benefit from measurements of the CO_2 levels above the brew to characterize the off-gassing dynamics in coffee brewing and their relation to coffee grounds sedimentation and concentration gradient.

One of the most surprising findings from our sensory work is that certain long time cold brews had similar sensory profiles to those of some short time hot brews, suggesting the sensory profiles of certain hot brews and cold brews could possibly be matched through controlled preparation of roast level, brew time, and serving temperature. Yet, our results indicated that this finding is roast dependent. To rigorously validate this point, it will be necessary to conduct discrimination tests to compare long-time-cold-brew and short-time-hot-brew coffee from a wider range of pre-brewing conditions including origins/processing methods and roast levels.

Another important aspect worth exploring in more detail is the serving temperature as it effects the sensory perception in coffee beverages (Adhikari et al., 2018; Chapko and Seo, 2019). All the coffees examined in our descriptive analysis were served cold to the panelists. A valuable direction to advance the understanding of how flavors evolve in full immersion brewing is to further investigate the sensory profiles in hot full immersion brew over time at a more frequent sampling intervals, similar to the fractionation descriptive analysis done for hot drip brew coffee (Batali et al., 2020a). Because our results for grind size and agitation are useful tools for fine-tuning the extraction dynamics, sensory analysis in regard to the change in these brewing parameters will also be of practical importance.

Our work focused on sensory descriptive analysis, but an equally important aspect is the consumer hedonic response to the cup. A follow-up study could explore hedonic testing with coffee consumers. An indirect approach like external preference mapping could be taken to link hedonic liking to sensory properties based on the descriptive analysis data of full immersion coffee. Following the idea of sensory engineering and Kansei engineering (Moskowitz, 1979; Nagamachi, 1995), preference maximizations of consumer clusters could be modeled and predicted based on sensory profiles, which subsequently allows trace back into how actionable brewing parameters affect the desirable flavor profiles for different consumers.

As sensory and consumer studies have shown, different consumers prefer different coffee flavor profiles (Cotter et al., 2021; Guinard et al., 2023). The coffee industry is moving away from the one-size-fits-all “ideal” belief about how coffee should be brewed, to a more consumer-centric brewing concept where different brewing profiles satisfy different tastes. Along with the established work in pursuing quality in coffee brewing, we hope this work and future studies will add new value and open new opportunities in using full immersion brewing methods to help the coffee industry achieve this goal for coffee-drinking consumers.

References

Adhikari, J., Chambers, E., Koppel, K., 2018. Impact of consumption temperature on sensory properties of hot brewed coffee. Food Res. Int. doi:10.1016/j.foodres.2018.08.014

Ahmed, M., Jiang, G.-H., Park, J.S., Lee, K.-C., Seok, Y.Y., Eun, J.B., 2019. Effects of ultrasonication, agitation and stirring extraction techniques on the physicochemical properties, health-promoting phytochemicals and structure of cold-brewed coffee. J. Sci. Food Agric. 99, 290–301. doi:10.1002/jsfa.9186

Akiyama, M., Murakami, K., Ohtani, N., Iwatsuki, K., Sotoyama, K., Wada, A., Tokuno, K., Iwabuchi, H., Tanaka, K., 2003. Analysis of volatile compounds released during the grinding of roasted coffee beans using solid-phase microextraction. J. Agric. Food Chem. 51, 1961–1969. doi:10.1021/jf020724p

Amidon, G.E., Meyer, P.J., Mudie, D.M., 2017. Particle, powder, and compact characterization, in: Developing Solid Oral Dosage Forms. Elsevier, pp. 271–293. doi:10.1016/B978-0-12-802447-8.00010-8

Andueza, S., De Peña, M.P., Cid, C., 2003a. Chemical and sensorial characteristics of espresso coffee as affected by grinding and torrefacto roast. J. Agric. Food Chem. 51, 7034–7039. doi:10.1021/jf034628f

Andueza, S., Maeztu, L., Pascual, L., Ibáñez, C., de Peña, M.P., Cid, C., 2003b. Influence of extraction temperature on the final quality of espresso coffee. J. Sci. Food Agric. 83, 240–248. doi:10.1002/jsfa.1304

Andueza, S., Vila, M.A., Paz de Peña, M., Cid, C., 2007. Influence of coffee/water ratio on the final quality of espresso coffee. J. Sci. Food Agric. 87, 586–592. doi:10.1002/jsfa.2720

Angeloni, G., Guerrini, L., Masella, P., Bellumori, M., Daluiso, S., Parenti, A., Innocenti, M., 2019a. What kind of coffee do you drink? An investigation on effects of eight different extraction methods. Food Res. Int. 116, 1327–1335. doi:10.1016/j.foodres.2018.10.022

Angeloni, G., Guerrini, L., Masella, P., Innocenti, M., Bellumori, M., Parenti, A., 2019b. Characterization and comparison of cold brew and cold drip coffee extraction methods. J. Sci. Food Agric. 99, 391–399. doi:10.1002/jsfa.9200

Batali, M.E., Cotter, A.R., Frost, S.C., Ristenpart, W.D., Guinard, J.-X., 2021. Titratable acidity, perceived sourness, and liking of acidity in drip brewed coffee. ACS Food Sci. Technol. doi:10.1021/acsfoodscitech.0c00078

Batali, M.E., Frost, S.C., Lebrilla, C.B., Ristenpart, W.D., Guinard, J.-X., 2020a. Sensory and monosaccharide analysis of drip brew coffee fractions versus brewing time. J. Sci. Food Agric. 100, 2953–2962. doi:10.1002/jsfa.10323

Batali, M.E., Lim, L.X., Liang, J., Yeager, S.E., Thompson, A.N., Han, J., Ristenpart, W.D., Guinard, J.-X., 2022. Sensory analysis of full immersion coffee: cold brew is more floral, and less bitter, sour, and rubbery than hot brew. Foods 11, 2440. doi:10.3390/foods11162440

Batali, M.E., Ristenpart, W.D., Guinard, J.-X., 2020b. Brew temperature, at fixed brew strength and extraction, has little impact on the sensory profile of drip brew coffee. Sci. Rep. 10, 16450. doi:10.1038/s41598-020-73341-4

Bekedam, E.K., Loots, M.J., Schols, H.A., Van Boekel, M.A.J.S., Smit, G., 2008. Roasting effects on formation mechanisms of coffee brew melanoidins. J. Agric. Food Chem. 56, 7138–7145. doi:10.1021/jf800999a

Bhumiratana, N., Adhikari, K., Chambers, E., 2011. Evolution of sensory aroma attributes from coffee beans to brewed coffee. LWT - Food Science and Technology 44, 2185–2192. doi:10.1016/j.lwt.2011.07.001

Borrelli, R.C., Visconti, A., Mennella, C., Anese, M., Fogliano, V., 2002. Chemical characterization and antioxidant properties of coffee melanoidins. J. Agric. Food Chem. 50, 6527–6533. doi:10.1021/jf025686o

Bustos-Vanegas, J.D., Corrêa, P.C., Martins, M.A., Baptestini, F.M., Campos, R.C., de Oliveira, G.H.H., Nunes, E.H.M., 2018. Developing predictive models for determining physical properties of coffee beans during the roasting process. Ind. Crops Prod. 112, 839–845. doi:10.1016/j.indcrop.2017.12.015

Cameron, M.I., Morisco, D., Hofstetter, D., Uman, E., Wilkinson, J., Kennedy, Z.C., Fontenot, S.A., Lee, W.T., Hendon, C.H., Foster, J.M., 2020. Systematically Improving Espresso: Insights from Mathematical Modeling and Experiment. Matter. doi:10.1016/j.matt.2019.12.019

Castañeda-Rodríguez, R., Mulík, S., Ozuna, C., 2020. Brewing temperature and particle size affect extraction kinetics of cold brew coffee in terms of its physicochemical, bioactive, and antioxidant properties. Journal of Culinary Science & Technology 1–22. doi:10.1080/15428052.2020.1848683

Chapko, M.J., Seo, H.-S., 2019. Characterizing product temperature-dependent sensory perception of brewed coffee beverages: Descriptive sensory analysis. Food Res. Int. 121, 612–621. doi:10.1016/j.foodres.2018.12.026

Clarke, R.J., Macrae, R. (Eds.), 1987. Coffee. Elsevier Science Publishers Ltd.

Coffee Quality Institute, 2022. Coffee Quality Institute Annual Report. Coffee Quality Institue.

Coffee Review, n.d. Coffee Review - Understanding roast definitions for coffee.

Cordoba, N., Fernandez-Alduenda, M., Moreno, F.L., Ruiz, Y., 2020. Coffee extraction: A review of parameters and their influence on the physicochemical characteristics and flavour of coffee brews. Trends Food Sci. Technol. 96, 45–60. doi:10.1016/j.tifs.2019.12.004

Córdoba, N., Moreno, F.L., Osorio, C., Velásquez, S., Ruiz, Y., 2021. Chemical and sensory evaluation of cold brew coffees using different roasting profiles and brewing methods. Food Res. Int. 141, 110141. doi:10.1016/j.foodres.2021.110141

Cordoba, N., Pataquiva, L., Osorio, C., Moreno, F.L.M., Ruiz, R.Y., 2019. Effect of grinding, extraction time and type of coffee on the physicochemical and flavour characteristics of cold brew coffee. Sci. Rep. 9, 8440. doi:10.1038/s41598-019-44886-w

Corrochano, B.R., Melrose, J.R., Bentley, A.C., Fryer, P.J., Bakalis, S., 2015. A new methodology to estimate the steady-state permeability of roast and ground coffee in packed beds. J. Food Eng. 150, 106–116. doi:10.1016/j.jfoodeng.2014.11.006

Costa Freitas, A.M., Mosca, A.I., 1999. Coffee geographic origin — an aid to coffee differentiation. Food Res. Int 32, 565–573. doi:10.1016/S0963-9969(99)00132-5

Cotter, A., Hopfer, H., 2018. The Effects of Storage Temperature on the Aroma of Whole Bean Arabica Coffee Evaluated by Coffee Consumers and HS-SPME-GC-MS. Beverages 4, 68. doi:10.3390/beverages4030068

Cotter, A.R., Batali, M.E., Ristenpart, W.D., Guinard, J.-X., 2021. Consumer preferences for black coffee are spread over a wide range of brew strengths and extraction yields. J. Food Sci. 86, 194–205. doi:10.1111/1750-3841.15561

De Bruyn, F., Zhang, S.J., Pothakos, V., Torres, J., Lambot, C., Moroni, A.V., Callanan, M., Sybesma, W., Weckx, S., De Vuyst, L., 2017. Exploring the Impacts of Postharvest Processing on the Microbiota and Metabolite Profiles during Green Coffee Bean Production. Appl. Environ. Microbiol. 83. doi:10.1128/AEM.02398-16

De Maria, C.A.B., Trugo, L.C., Moreira, R.F.A., Werneck, C.C., 1994. Composition of green coffee fractions and their contribution to the volatile profile formed during roasting. Food Chem. 50, 141–145. doi:10.1016/0308-8146(94)90111-2

Di Donfrancesco, B., Gutierrez Guzman, N., Chambers, E., 2014. Comparison of Results from Cupping and Descriptive Sensory Analysis of Colombian Brewed Coffee. J Sens Stud 29, 301–311. doi:10.1111/joss.12104

Elhalis, H., Cox, J., Zhao, J., 2023. Coffee fermentation: Expedition from traditional to controlled process and perspectives for industrialization. Applied Food Research 3, 100253. doi:10.1016/j.afres.2022.100253

Emadzadeh, A., Chiew, Y.-M., 2020. Settling velocity of porous spherical particles. J. Hydraul. Eng. 146, 04019046. doi:10.1061/(ASCE)HY.1943-7900.0001655

Espinoza-Pérez, J.D., Vargas, A., Robles-Olvera, V.J., Rodrı´guez-Jimenes, G.C., Garcı´a-Alvarado, M.A., 2007. Mathematical modeling of caffeine kinetic during solid–liquid extraction of coffee beans. J. Food Eng. 81, 72–78. doi:10.1016/j.jfoodeng.2006.10.011

Fasano, A., Talamucci, F., 2000. A comprehensive mathematical model for a multispecies flow through ground coffee. SIAM J. Math. Anal. 31, 251–273. doi:10.1137/S0036141098336698

Feria-Morales, A.M., 2002. Examining the case of green coffee to illustrate the limitations of grading systems/expert tasters in sensory evaluation for quality control. Food Qual

Prefer 13, 355–367. doi:10.1016/S0950-3293(02)00028-9

Fioresi, D.B., Ramos, A.C., Bertolazi, A.A., Pereira, L.L., 2023. Adherence and concordance amongQ-Graders in the sensory analysis of coffees. J Sens Stud 38. doi:10.1111/joss.12805

Fogler, H., 2020. Elements of Chemical Reaction Engineering (International Series in the Physical and Chemical Engineering Sciences), 6th ed. Pearson, Boston.

Frost, S.C., Ristenpart, W.D., Guinard, J.-X., 2019. Effect of basket geometry on the sensory quality and consumer acceptance of drip brewed coffee. J. Food Sci. 84, 2297–2312. doi:10.1111/1750-3841.14696

Frost, S.C., Ristenpart, W.D., Guinard, J.-X., 2020. Effects of brew strength, brew yield, and roast on the sensory quality of drip brewed coffee. J. Food Sci. 85, 2530–2543. doi:10.1111/1750-3841.15326

Fuller, M., Rao, N.Z., 2017. The effect of time, roasting temperature, and grind size on caffeine and chlorogenic acid concentrations in cold brew coffee. Sci. Rep. 7, 17979. doi:10.1038/s41598-017-18247-4

Gloess, A.N., Schönbächler, B., Klopprogge, B., D`Ambrosio, L., Chatelain, K., Bongartz, A., Strittmatter, A., Rast, M., Yeretzian, C., 2013. Comparison of nine common coffee extraction methods: instrumental and sensory analysis. Eur. Food Res. Technol. 236, 607–627. doi:10.1007/s00217-013-1917-x

Gloess, A.N., Vietri, A., Wieland, F., Smrke, S., Schönbächler, B., López, J.A.S., Petrozzi, S., Bongers, S., Koziorowski, T., Yeretzian, C., 2014. Evidence of different flavour formation dynamics by roasting coffee from different origins: On-line analysis with PTR-ToF-MS.

Int. J. Mass Spectrom. 365–366, 324–337. doi:10.1016/j.ijms.2014.02.010

Guinard, J.-X., Frost, S., Batali, M., Cotter, A., Lim, L.X., Ristenpart, W.D., 2023. A new Coffee Brewing Control Chart relating sensory properties and consumer liking to brew strength, extraction yield, and brew ratio. J. Food Sci. 88, 2168–2177. doi:10.1111/1750-3841.16531

Hargarten, V.B., Kuhn, M., Briesen, H., 2020. Swelling properties of roasted coffee particles. J. Sci. Food Agric. 100, 3960–3970. doi:10.1002/jsfa.10440

Harwood, W.S., McLean, K.G., Ennis, J.M., Ennis, D.M., Drake, M., 2020. Comparison of preference mapping with projective mapping for characterizing consumer perception of brewed black coffees. J Sens Stud 35. doi:10.1111/joss.12563

Herrera, J.C., Lambot, C., 2017. The coffee tree—genetic diversity and origin, in: The Craft and Science of Coffee. Elsevier, pp. 1–16. doi:10.1016/B978-0-12-803520-7.00001-3

Hoffmann, J., 2018. The World Atlas of Coffee, 2nd ed. Firefly Books.

International Coffee Organization, 2023. Coffee Market Report. Internaltional Coffee Organization (ICO).

Jaganyi, D., Madlala, S.P., 2000. Kinetics of coffee infusion: a comparative study on the extraction kinetics of mineral ions and caffeine from several types of medium roasted coffees. Journal of the Science of Food and Agriculture.

Lee, H.S., O'Mahony, M., 2002. At what temperatures do consumers like to drink coffee?: mixing methods. J. Food Sci. 67, 2774–2777. doi:10.1111/j.1365-2621.2002.tb08814.x

Lee, L.W., Cheong, M.W., Curran, P., Yu, B., Liu, S.Q., 2015. Coffee fermentation and flavor--An intricate and delicate relationship. Food Chem. 185, 182–191.

doi:10.1016/j.foodchem.2015.03.124

Lee, T.A., Kempthorne, R., Hardy, J.K., 1992. Compositional changes in brewed coffee as a function of brewing time. J. Food Sci. 57, 1417–1419. doi:10.1111/j.1365-2621.1992.tb06872.x

Liang, J., Brown, H., Dunkin, M., Ristenpart, W.D., 2023. Concentration gradient inversion via sedimentation of coffee grounds in full immersion brewing. J. Food Eng. 111619. doi:10.1016/j.jfoodeng.2023.111619

Liang, J., Chan, K.C., Ristenpart, W.D., 2021. An equilibrium desorption model for the strength and extraction yield of full immersion brewed coffee. Sci. Rep. 11, 6904. doi:10.1038/s41598-021-85787-1

Liang, J., Lim, L.X., Weber, A.L., Han, J., Batali, M.E., Ristenpart, W.D., n.d. An Updated Diffusion-Limited Model for the Extraction Dynamics of Full Immersion Brewed Coffee: Impact of Temperature, Roast Level, and Origin.

Lingle, T.R., 2011. The coffee brewing handbook : a systematic guide to coffee preparation. Specialty Coffee Association of America.

Lingle, T.R., Menon, S.N., 2017. Cupping and Grading—Discovering Character and Quality, in: The Craft and Science of Coffee. Elsevier, pp. 181–203. doi:10.1016/B978-0-12-803520-7.00008-6

Lockhart, E.E., Pan American Coffee Bureau, National Coffee Association of U.S.A., 1957. The soluble solids in beverage coffee as an index to cup quality. Coffee Brewing Institute, New York.

Maille, M.J., Sala, K., Scott, D.M., Zukswert, H., 2021. Critical examination of particle swelling during wetting of ground coffee. J. Food Eng. 295, 110420. doi:10.1016/j.jfoodeng.2020.110420

Martins, P.M.M., Batista, N.N., Miguel, M.G. da C.P., Simão, J.B.P., Soares, J.R., Schwan, R.F., 2020. Coffee growing altitude influences the microbiota, chemical compounds and the quality of fermented coffees. Food Res. Int. 129, 108872. doi:10.1016/j.foodres.2019.108872

Melrose, J., Roman-Corrochano, B., Montoya-Guerra, M., Bakalis, S., 2018. Toward a new brewing control chart for the 21st century. J. Agric. Food Chem. 66, 5301–5309. doi:10.1021/acs.jafc.7b04848

Mestdagh, F., Davidek, T., Chaumonteuil, M., Folmer, B., Blank, I., 2014. The kinetics of coffee aroma extraction. Food Res. Int 63, 271–274. doi:10.1016/j.foodres.2014.03.011

Mestdagh, F., Glabasnia, A., Giuliano, P., 2017. The brew—extracting for excellence, in: The Craft and Science of Coffee. Elsevier, pp. 355–380. doi:10.1016/B978-0-12-803520-7.00015-3

Mintel, 2017. US coffee house sales expected to reach $28.7 billion by 2021 [WWW Document]. URL https://www.mintel.com/press-centre/us-coffee-house-sales-expected-to-reach-28-7-billion-by-2021/ (accessed 7.21.23).

Mitterlehner, M., Danninger, H., Gierl-Mayer, C., Gschiel, H., Martinez, C., Tomisser, M., Schatz, M., Senck, S., Auer, J., Benigni, C., 2021. Comparative evaluation of characterization methods for powders used in additive manufacturing. J Mater Eng Perform 30, 7019–7034. doi:10.1007/s11665-021-06113-4

Mo, C., Navarini, L., Liverani, F.S., Ellero, M., 2022. Modeling swelling effects during coffee extraction with smoothed particle hydrodynamics. Phys. Fluids 34, 043104. doi:10.1063/5.0086897

Moroney, K.M., Lee, W.T., O'Brien, S.B.G., Suijver, F., Marra, J., 2015. Modelling of coffee extraction during brewing using multiscale methods: An experimentally validated model. Chem Eng Sci 137, 216–234. doi:10.1016/j.ces.2015.06.003

Moroney, K.M., Lee, W.T., O'Brien, S.B.G., Suijver, F., Marra, J., 2016. Coffee extraction kinetics in a well mixed system. J.Math.Industry 7, 3. doi:10.1186/s13362-016-0024-6

Moroney, K.M., O'Connell, K., Meikle-Janney, P., O'Brien, S.B.G., Walker, G.M., Lee, W.T., 2019. Analysing extraction uniformity from porous coffee beds using mathematical modelling and computational fluid dynamics approaches. PLoS One 14, e0219906. doi:10.1371/journal.pone.0219906

Moskowitz, H.R., 1979. Odor psychophysics and sensory engineering. Chem. Senses 4, 163–174. doi:10.1093/chemse/4.2.163

Nagamachi, M., 1995. Kansei Engineering: A new ergonomic consumer-oriented technology for product development. Int J Ind Ergon 15, 3–11. doi:10.1016/0169-8141(94)00052-5

Nakilcioğlu-Taş, E., Ötleş, S., 2019. Physical characterization of Arabica ground coffee with different roasting degrees. An. Acad. Bras. Cienc 91, e20180191. doi:10.1590/0001-3765201920180191

Nestlé Waters North America, Inc., 2019. Nestlé Pure Life® 2019 Water Analysis Report . Nestlé Waters North America, Inc.,.

Nestlé Waters North America, Inc., 2021. Nestlé Pure Life® Quality Reports, 19 L Analysis Report. Nestlé Waters North America, Inc.,.

Ortolá, M.D., Londoño, L., Gutiérrez, C.L., Chiralt, A., 1998. Influence of roasting temperature on physicochemical properties of different coffees. Food Science and Technology International 4, 59–66. doi:10.1177/108201329800400108

Pereira, L.L., Cardoso, W.S., Guarçoni, R.C., da Fonseca, A.F.A., Moreira, T.R., Caten, C.S. ten, 2017. The consistency in the sensory analysis of coffees using Q-graders. Eur. Food Res. Technol. 243, 1545–1554. doi:10.1007/s00217-017-2863-9

Pereira, L.L., Guarçoni, R.C., Pinheiro, P.F., Osório, V.M., Pinheiro, C.A., Moreira, T.R., Ten Caten, C.S., 2020. New propositions about coffee wet processing: Chemical and sensory perspectives. Food Chem. 310, 125943. doi:10.1016/j.foodchem.2019.125943

Pérez-Martínez, M., Sopelana, P., de Peña, M.P., Cid, C., 2008. Changes in volatile compounds and overall aroma profile during storage of coffee brews at 4 and 25 degrees C. J. Agric. Food Chem. 56, 3145–3154. doi:10.1021/jf703731x

Pinsuwan, A., Suwonsichon, S., Chompreeda, P., Prinyawiwatkul, W., 2022. Sensory Drivers of Consumer Acceptance, Purchase Intent and Emotions toward Brewed Black Coffee. Foods 11. doi:10.3390/foods11020180

Portela, C. da S., Almeida, I.F. de, Mori, A.L.B., Yamashita, F., Benassi, M. de T., 2021. Brewing conditions impact on the composition and characteristics of cold brew Arabica and Robusta coffee beverages. LWT 143, 111090. doi:10.1016/j.lwt.2021.111090

Portela, C. da S., Almeida, I.F. de, Reis, T.A.D.D., Hickmann, B.R.B., Benassi, M. de T., 2022. Effects of brewing conditions and coffee species on the physicochemical characteristics, preference and dynamics of sensory attributes perception in cold brews. Food Res. Int. 151, 110860. doi:10.1016/j.foodres.2021.110860

Price, W.E., 1989. Tracer caffeine diffusion in aqueous solutions at 298 K. The effect of caffeine self-association. J. Chem. Soc., Faraday Trans. 1 85, 415. doi:10.1039/f19898500415

Ramalakshmi, K., Raghavan, B., 1999. Caffeine in coffee: its removal. Why and how? Crit. Rev. Food Sci. Nutr. 39, 441–456. doi:10.1080/10408699991279231

Rao, N.Z., Fuller, M., Grim, M.D., 2020. Physiochemical characteristics of hot and cold brew coffee chemistry: the effects of roast level and brewing temperature on compound extraction. Foods 9. doi:10.3390/foods9070902

Redgwell, R.J., Trovato, V., Curti, D., Fischer, M., 2002. Effect of roasting on degradation and structural features of polysaccharides in Arabica coffee beans. Carbohydr. Res. 337, 421–431. doi:10.1016/S0008-6215(02)00010-1

Ristenpart, W.D., Kuhl, T., 2017. The Design of Coffee: An Engineering Apporach.

Rostagno, M.A., Celeghini, R.M.S., Debien, I.C.N., Nogueira, G.C., Meireles, M.A.A., 2015. Phenolic compounds in coffee compared to other beverages, in: Coffee in Health and Disease Prevention. Elsevier, pp. 137–142. doi:10.1016/B978-0-12-409517-5.00015-2

Rotta, N.M., Curry, S., Han, J., Reconco, R., Spang, E., Ristenpart, W., Donis-González, I.R., 2021. A comprehensive analysis of operations and mass flows in postharvest processing of washed coffee. Resources, Conservation and Recycling 170, 105554. doi:10.1016/j.resconrec.2021.105554

Rufián-Henares, J.A., Pastoriza, S., 2015. Melanoidins in Coffee, in: Coffee in Health and Disease Prevention. Elsevier, pp. 183–188. doi:10.1016/B978-0-12-409517-5.00020-6

Samoggia, A., Riedel, B., 2018. Coffee consumption and purchasing behavior review: Insights for further research. Appetite 129, 70–81. doi:10.1016/j.appet.2018.07.002

Schenker, S., Handschin, S., Frey, B., Perren, R., Escher, F., 2000. Pore structure of coffee beans affected by roasting conditions. J. Food Sci. 65, 452–457. doi:10.1111/j.1365-2621.2000.tb16026.x

Schneider, C.A., Rasband, W.S., Eliceiri, K.W., 2012. NIH Image to ImageJ: 25 years of image analysis. Nat. Methods 9, 671–675. doi:10.1038/nmeth.2089

Scholz, M.B. dos S., Prudencio, S.H., Kitzberger, C.S.G., Silva, R.S. dos S.F. da, 2019. Physico-chemical characteristics and sensory attributes of coffee beans submitted to two post-harvest processes. Food Measure. 13, 831–839. doi:10.1007/s11694-018-9995-x

Seninde, D.R., Chambers, E., Chambers, D., 2020. Determining the impact of roasting degree, coffee to water ratio and brewing method on the sensory characteristics of cold brew Ugandan coffee. Food Res. Int. 137, 109667. doi:10.1016/j.foodres.2020.109667

Severini, C., Ricci, I., Marone, M., Derossi, A., De Pilli, T., 2015. Changes in the aromatic profile of espresso coffee as a function of the grinding grade and extraction time: a study by the electronic nose system. J. Agric. Food Chem. 63, 2321–2327. doi:10.1021/jf505691u

Smrke, S., Wellinger, M., Suzuki, T., Balsiger, F., Opitz, S.E.W., Yeretzian, C., 2018. Time-Resolved Gravimetric Method To Assess Degassing of Roasted Coffee. J. Agric. Food Chem. 66, 5293–5300. doi:10.1021/acs.jafc.7b03310

Specialty Coffee Association, 2018. Coffee Standard. Specialty Coffee Association.

Specialty Coffee Association, 2019. US Coffee Market Overview 2018. Specialty Coffee Association.

Specialty Coffee Association, 2021. Towards a Definition of Specialty Coffee: Building an Understanding Based on Attributes. Specialty Coffee Association.

Specialty Coffee Association, 2022. Understanding and Evolving the SCA Coffee Value Assessment System: Results of the 2020-2021 Cupping Protocol User Perception Study and Proposed Evolution. Specialty Coffee Association.

Specialty Coffee Association, n.d. Protocols & Best Practices — Specialty Coffee Association [WWW Document]. URL https://sca.coffee/research/protocols-best-practices?page=resources&d=cupping-protocols (accessed 1.20.22).

Spencer, M., Sage, E., Velez, M., Guinard, J.-X., 2016. Using single free sorting and multivariate exploratory methods to design a new coffee taster's flavor wheel. J. Food Sci. 81, S2997–S3005. doi:10.1111/1750-3841.13555

Spiro, M., 1993. Modelling the aqueous extraction of soluble substances from ground roast coffee. J. Sci. Food Agric. 61, 371–372. doi:10.1002/jsfa.2740610314

Spiro, M., Chong, Y.Y., 1997. The Kinetics and Mechanism of Caffeine Infusion from Coffee: the Temperature Variation of the Hindrance Factor. J. Sci. Food Agric. 74, 416–420. doi:10.1002/(SICI)1097-0010(199707)74:3<416::AID-JSFA868>3.0.CO;2-0

Spiro, M., Hunter, J.E., 1985. The kinetics and mechanism of caffeine infusion from coffee: The effect of roasting. J. Sci. Food Agric. 36, 871–876. doi:10.1002/jsfa.2740360917

Spiro, M., Page, C.M., 1984. The Kinetics and mechanism of caffeine infusion from coffee: Hydrodynamic aspects. J. Sci. Food Agric. 35, 925–930. doi:10.1002/jsfa.2740350818

Spiro, M., Selwood, R.M., 1984. The kinetics and mechanism of caffeine infusion from coffee: The effect of particle size. J. Sci. Food Agric. 35, 915–924. doi:10.1002/jsfa.2740350817

Spiro, M., Toumi, R., Kandiah, M., 1989. The kinetics and mechanism of caffeine infusion from coffee: The hindrance factor in intra-bean diffusion. J. Sci. Food Agric. 46, 349–356.

doi:10.1002/jsfa.2740460313

Stapley, A.G., 2002. Modelling the kinetics of tea and coffee infusion. J. Sci. Food Agric. 82, 1661–1671. doi:10.1002/jsfa.1250

Sualeh, A., Tolessa, K., Mohammed, A., 2020. Biochemical composition of green and roasted coffee beans and their association with coffee quality from different districts of southwest Ethiopia. Heliyon 6, e05812. doi:10.1016/j.heliyon.2020.e05812

Sunarharum, W.B., Williams, D.J., Smyth, H.E., 2014. Complexity of coffee flavor: A compositional and sensory perspective. Food Res. Int 62, 315–325. doi:10.1016/j.foodres.2014.02.030

The National Coffee Association of USA, 2023. 2023 National Coffee Data Trends Specialty Coffee Report.

Tian, T., Freeman, S., Corey, M., German, J.B., Barile, D., 2018. Effect of roasting on oligosaccharide abundance in arabica coffee beans. J. Agric. Food Chem. 66, 10067–10076. doi:10.1021/acs.jafc.8b02641

Toddy, 2020. Recommended Protocols: Cold Brew Cupping [WWW Document]. URL https://toddycafe.com/ (accessed 3.28.23).

Traore, T.M., Wilson, N.L.W., Fields, D., 2018. What explains specialty coffee quality scores and prices: a case study from the cup of excellence program. J. agric. appl. econ. 50, 349–368. doi:10.1017/aae.2018.5

Uman, E., Colonna-Dashwood, M., Colonna-Dashwood, L., Perger, M., Klatt, C., Leighton, S., Miller, B., Butler, K.T., Melot, B.C., Speirs, R.W., Hendon, C.H., 2016. The effect of bean origin and temperature on grinding roasted coffee. Sci. Rep. 6, 24483.

doi:10.1038/srep24483

van der Merwe, K., Maree, T., 2016. The behavioural intentions of specialty coffee consumers in South Africa. Int. J. Consum. Stud. 40, 501–508. doi:10.1111/ijcs.12275

Vezzulli, F., Rocchetti, G., Lambri, M., Lucini, L., 2022. Metabolomics Combined with Sensory Analysis Reveals the Impact of Different Extraction Methods on Coffee Beverages from Coffea arabica and Coffea canephora var. Robusta. Foods 11, 807. doi:10.3390/foods11060807

Voilley, A., Simatos, D., 1979. Modeling the solubilization process during coffee brewing. J. Food Process Eng. 3, 185–198. doi:10.1111/j.1745-4530.1979.tb00238.x

Wadsworth, F.B., Vossen, C.E.J., Heap, M.J., Kushnir, A., Farquharson, J.I., Schmid, D., Dingwell, D.B., Belohlavek, L., Huebsch, M., Carbillet, L., Kendrick, J.E., 2021. The force required to operate the plunger on a French press. Am J Phys 89, 769–775. doi:10.1119/10.0004224

Wang, X., Lim, L., 2021. Modeling study of coffee extraction at different temperature and grind size conditions to better understand the cold and hot brewing process. J. Food Process Eng. doi:10.1111/jfpe.13748

Wang, X., Lim, L.-T., 2014. Effect of roasting conditions on carbon dioxide degassing behavior in coffee. Food Res. Int 61, 144–151. doi:10.1016/j.foodres.2014.01.027

Wei, F., Tanokura, M., 2015. Chemical Changes in the Components of Coffee Beans during Roasting, in: Coffee in Health and Disease Prevention. Elsevier, pp. 83–91. doi:10.1016/B978-0-12-409517-5.00010-3

Welty, J., Rorrer, G.L., Foster, D.G., 2014. Fundamentals of Momentum, Heat and Mass Transfer, 6th ed. Wiley Global Education US.

Yeager, S.E., Batali, M.E., Guinard, J.-X., Ristenpart, W.D., 2021. Acids in coffee: A review of sensory measurements and meta-analysis of chemical composition. Crit. Rev. Food Sci. Nutr. 63, 1010–1036. doi:10.1080/10408398.2021.1957767

Yeager, S.E., Batali, M.E., Lim, L.X., Liang, J., Han, J., Thompson, A.N., Guinard, J.-X., Ristenpart, W.D., 2022. Roast level and brew temperature significantly affect the color of brewed coffee. J. Food Sci. 87, 1837–1850. doi:10.1111/1750-3841.16089

Zanoni, B., Pagliarini, E., Peri, C., 1992. Modelling the aqueous extraction of soluble substances from ground roasted coffee. J. Sci. Food Agric. 58, 275–279. doi:10.1002/jsfa.2740580217

Zhang, S.J., De Bruyn, F., Pothakos, V., Contreras, G.F., Cai, Z., Moccand, C., Weckx, S., De Vuyst, L., 2019a. Influence of various processing parameters on the microbial community dynamics, metabolomic profiles, and cup quality during wet coffee processing. Front. Microbiol. 10, 2621. doi:10.3389/fmicb.2019.02621

Zhang, S.J., De Bruyn, F., Pothakos, V., Torres, J., Falconi, C., Moccand, C., Weckx, S., De Vuyst, L., 2019b. Following Coffee Production from Cherries to Cup: Microbiological and Metabolomic Analysis of Wet Processing of Coffea arabica. Appl. Environ. Microbiol. 85. doi:10.1128/AEM.02635-18