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Titratable Acidity, Perceived Sourness, and Liking of Acidity in Drip Brewed Coffee

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ABSTRACT: Acidity is a highly prized attribute in coffee, but there is little understanding of the brewing conditions under which acidity contributes favorable sensory attributes versus unfavorable sourness. Here, we examine the effect of titratable acidity and pH on the perception of sourness and consumer acceptance in drip brew coffee. Sour perception and acidity liking were assessed over a wide range of brew strengths and extraction yields at three different roast levels (light, medium, dark) and three different brewing temperatures (87 °C, 90 °C, and 93 °C). We find that perceived sour intensity correlates weakly with pH, but strongly with titratable acidity. Increases in titratable acidity also yielded increases in consumer perception of "too much acidity" and also impacted consumer liking and consumer preference segmentation with one cluster of consumers preferring more acidic coffee. Importantly, our data show that titratable acidity is linearly correlated with total dissolved solids (TDS) under all conditions studied, indicating that TDS is a good proxy for titratable acidity. The results presented here will provide the coffee industry with insight toward controlling perceived acidity or sourness, a key sensory attribute that substantially impacts consumer acceptance.

KEYWORDS: *coffee, sensory analysis, consumer preference, extraction, coffee brewing, organic acids*

1. INTRODUCTION

When experts score coffee through the traditional method known as "cupping", perception of acidity is 1 of 10 main components that can increase or decrease coffee quality scores.[1] According to the "cupping best practices" published by the Specialty Coffee Association:

"Acidity is often described as "brightness" when favorable or "sour" when unfavorable. At its best, acidity contributes to a coffee's liveliness, sweetness, and fresh-fruit character and is almost immediately experienced and evaluated when the coffee is first slurped into the mouth. Acidity that is overly intense or dominating may be unpleasant, however, and excessive acidity may not be appropriate to the flavor profile of the sample."[2]

Not only is acidity scored separately but perceived acidity or sourness is also mentioned as a component of other cupping score categories, including flavor, balance, and defects, and likely contributes to uniformity and overall score as well.[2] While the popularity of coffee is driven in part by its caffeine content, it is a complex blend of nonvolatile and volatile compounds that contribute to its sensory appeal.[3] Many different acids can be found in brewed coffee, with a variety of organic acids in the brew potentially impacting coffee flavor.[4] The Coffee Taster's Flavor Wheel presents 104 different attributes in coffee that may contribute to the overall sensory profile, and about 10% of these could be clearly linked to acids from positive attributes like Citrus-Grapefruit to potentially negative attributes like Sour-Butyric Acid.[5] Understanding how chemical content of acids links to sensory perception of acids will better inform the industry's understanding of coffee sensory qualities.

Green coffee is about 8−10% acid by mass, including both aliphatic acids and chlorogenic acids.[6] Aliphatic acids present in green coffee include citric, malic, and lactic acid; upon roasting the citric and malic acid undergo degradation into succinic, fumaric, and maleic acid, while acetic formic, lactic, and glycolic acid form from hydrolysis of various carbohydrates.[6] Chlorogenic acids contribute to antioxidant activity[7] and decrease in concentration as they react to form bitter chlorogenic acid lactones during roasting.[8] Although some acids form during roasting and some acids break down, overall the acid content of coffee tends to decrease with darker roasts.[6]

Most of the smaller organic acids, such as citric, acetic, formic, malic, quinic, pyruvic, succinic, fumaric, tartaric, and lactic acid all are sour tasting acids, though some, such as acetic acid with its characteristic vinegar quality, will contribute to aroma as well.[9,10] However, not all acids contribute to typical "acidity" in the same way. Some aliphatic acids are also bitter, (formic, succinic, quinic, and caffeic),[8,10,11] and astringent (quinic and lactic).[9,10,12] Chlorogenic acids as well are generally more bitter and astringent than sour, and potentially metallic.[6,7,13] As such, it is important to consider that there might be a difference between chemical acidity and sensory acidity as evaluated by experts.

Although the green composition and roast profile clearly affect the acidity of the beans, it is the brewing step that governs the ultimate acidity and corresponding sensory qualities of the final beverage. Historically, there has been

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little insight as to the best brewing practices to optimize this acidity. For decades, the coffee industry has relied on the classic Coffee Brewing Control Chart (Figure 1) as a metric for coffee quality. The Coffee Brewing Control Chart comprises three key physical measurements. The "total dissolved solids" (TDS) represent the brew strength, expressed as the mass fraction of dissolved solids present in the beverage and typically measured via digital refractometry. Percent extraction (PE) refers to the extraction yield of the material in the original dry grounds ultimately extracted into the liquid phase during brewing and is typically measured either by an oven drying technique or by using mass conservation arguments to relate it to the TDS.[15] Finally, the brew ratio refers to the mass ratio of water to dry coffee grounds. The Coffee Brewing Control Chart shows the mass relationship between TDS, PE, and brew ratio and predicts sensory qualities and "ideal" extraction for brewed coffee based on these values.[14] In coffee brewing vocational training, the chart is a core metric for coffee quality with TDS and PE believed to be predictors of properties like "underdeveloped" (pealike, grassy, at low PE), "bitter" (at high PE), or "weak/strong" flavor (low/high TDS, respectively).[16]

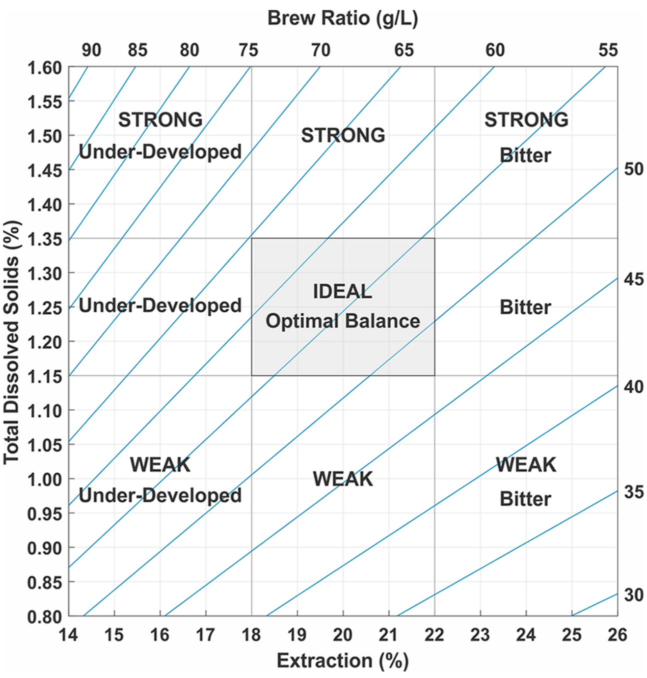

Figure 1. Classic Coffee Brewing Control Chart, originally developed by Lockhart.[14] Reproduced from Ristenpart and Kuhl, 2017.[15]

Previous work has clearly shown that differences in brewing will yield differences in TDS, PE, and the corresponding sensory profile for various brewing methods.[4,17−23] Recently, our group has performed systematic experiments with drip brews spanning the entire range of the Coffee Brewing Control Chart, yielding a wealth of sensory and consumer preference data.[20,21,23] In each set of investigations, coffees were brewed to three distinct levels of TDS (1.0%, 1.25%, and 1.5%), three distinct levels of PE (16%, 20%, 24%), and various roast levels or brew temperatures. Specifically, Frost et al.[20] used descriptive analysis to explore how specific sensory attributes changed across the Coffee Brewing Control Chart for three different roast levels of the same green coffee at the 9 extraction levels, systematically investigating 27 different TDS-PE-Roast combinations. Batali et al.[21] and Cotter et al.[23] performed further systematic descriptive analysis and consumer tests of coffee at a single roast level but brewed at the same 9 TDS-PE combinations with 3 different brewing temperatures (87 °C, 90 °C, and 93 °C), again yielding 27 sample types. Mapping trends across the Coffee Brewing Control Chart, we found that higher TDS coffee was consistently more bitter, astringent, and viscous, and low TDS coffee was more sweet, fruity, and tea-like/floral.[20,21] High TDS, low PE coffee was sour, citrusy, and fermented, and high TDS, high PE coffee was burnt, roasted, and ashy.[20,21] Consumer liking trends split consumers into two preference clusters, one being Cluster 2 who tended to prefer low TDS, sweeter coffee, and Cluster 1 who tended to prefer high and low PE coffee at higher levels of TDS.[23]

In both descriptive analysis studies,[20,21] we found that the trained panelists consistently found that "sour taste" exhibited the largest magnitude of change simply by brewing the same beans differently. High TDS, low PE coffee was perceived as most sour regardless of roast or brewing temperature, while low TDS, high PE coffee was perceived as least sour. This behavior was observed regardless of brew temperature or roast level, and no other sensory attribute had similarly large magnitudes of change universally across all evaluated coffees. Likewise, consumer evaluation by untrained panelists revealed that "acidity liking" changed drastically with brewing parameters with low PE, high TDS coffees more likely to be perceived as "too acidic" and high PE, low TDS coffees as "not acidic enough",[23] consistent with where the trained panelists detected much sourness or little sourness, respectively. Thus, both descriptive analysis and consumer preference testing indicates that understanding chemically how sourness is impacted by brewing could help coffee brewers more easily manipulate an attribute that will likely contribute heavily to perceived quality. These previous studies, however, did not provide any chemical measures of the acidity of the respective brews, so the correlation between acidity and perceived sourness and consumer liking remains unclear to date.

Some prior studies have used titratable acidity as one of multiple chemical measures to characterize differences between coffee samples with mixed results. In green coffee, higher titratable acidity has been shown to correlate with higher cup quality,[24] however this is likely due to reactions occurring with acids during roasting. Voilley et al. observed a correlation between acidity and TDS (expressed as "solid content" in their work), and a correlation between titratable acid and perceived acidity of coffees brewed at different temperatures and grinds.[25] In a more recent brewing study, Gloess et al. compared nine coffee extraction methods, including several types of espresso, lunghi, filter coffee, and French press and analyzed total solids, titratable acidity, and sensory profiles by consensus, among other factors, and found again that total solids were correlated to titratable acidity, but pH and titratable acidity did not correlate to perceived acidity.[17] At a larger range of titratable acidity, Fuse et al. likewise observed a correlation between titratable acidity of coffee and perceived sourness.[26] More recently, comparing sensory quality and chemical composition of novel roasting techniques, Kim et al. found that their novel "puffing" roasting techniques that had a higher extraction yield (percent extraction) also had a higher titratable acidity and were rated as more sour but that did not impact overall flavor acceptance or liking.[27] Lastly, in cold

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brew coffee the cold brew had a higher TDS but a lower titratable acidity and was also perceived as less acidic than hot brew coffees (though consumption temperature was not fixed).[22]

These studies strongly indicate that TA and sourness in coffee are linked but previous work to date has examined only limited ranges of TDS, PE, and other brew variables like temperature when measuring TA and sourness. Specifically, there currently is no guidance in format similar to the classic Coffee Brewing Control Chart to map TA and perceived sourness onto the brewing metrics of TDS and PE. In this paper, we collate the systematic sensory and consumer preference data previously reported in the three separates studies described above[20,21,23] and combine it with previously unreported chemical measurements of the pH and titratable acidity for all brews tested. We hypothesized that sensory measures of sourness or acidity would correlate with chemical measures of pH and titratable acidity, and in turn, that all measures of acidity (chemical acidity, sourness perceived by panel, and consumer liking of acidity) would correlate with the physical measurements of TDS and PE.

2. MATERIALS AND METHODS

All sensory and consumer liking data used in this work were previously collected as a part of larger descriptive and consumer analysis studies as referenced above.[20,21,23] Those three studies involved a total of 744 individual drip brews, all of which had their pH and titratable acidity measured individually as described below; these pH and TA data were not previously analyzed or reported. Here, we combine specific sourness and acidity perception data from the sensory studies with the measurements of pH and TA, yielding new correlations and new insights between the sensory data and the chemical data. We refer interested readers to references[20,21,23] for full methodology for the sensory experiments; here we provide only a brief overview and new details about chemical measurements of acidity and data analysis. For clarity, we henceforth refer to the sensory descriptive results presented by Frost et al.[20] as the "roast experiment", the sensory descriptive results presented by Batali et al.[21] as the "temperature experiment", and the consumer preference testing by Cotter et al.[23] as the "consumer experiment."

2.1. Overview. Roasted coffees were stored frozen and sealed until the night before experiments, where whole beans were allowed to reach room temperature before opening and grinding. Coffees were opened and ground immediately prior to brewing on a Mahlkonig Guatemala Lab Grinder. All coffees were brewed on a programmable Curtis G4 Single 1.0 Gal brewer (#G4TP1S63A3100, Wilbur Curtis Co., Montebello, CA). All coffees were brewed with reverse osmosis water prepared by dissolving 0.0116 g of $CaSO_4{\cdot}2H_2O$, 0.0497 g of $MgSO_4$, 0.0326 g of $NaHCO_3$, and 0.0257 g of $KHCO_3$ per liter of deioinized water and leaving the solution to equilibrate with ambient CO_2 as specified by industry standards.[28] Coffees in each experiment were brewed to a TDS of 1%, 1.25%, or 1.5% and a PE of 16%, 20%, or 24% for 9 TDS-PE combinations total. Coffees were brewed to the desired TDS and PE by altering grind size, brew ratio, water pulsing duty cycle, and number of water pulsing cycles. Variations in the water pulsing cycle increase the brew time, which ultimately allows for increased mass transfer from the grounds and increases TDS and PE. Detailed brew settings can be found in Table 1 of Frost et al.[20] and Table S1 of Batali et al.[21]

2.1.1. Roast Experiment. The same green coffee was roasted to three different levels, representing a typical "light", "medium", and "dark" roast by varying development time post first crack. The green coffee was a wet washed Arabica sourced from Siguatepeque, Comayagua, Honduras and roasted on a Loring S35 commercial roaster. Full roasting parameters were previously published by Frost et al.[20] Coffees were packaged in 1 lb. polypropylene bags with a one-way valve and heat sealed, then stored at −40 °C until brewed. The three roast levels were brewed to the 9 TDS-PE combinations for 27 sample types total. With replication and multiple tasting sessions to accommodate panelist schedules, 258 individual brews were evaluated.

Table 1. Means by Roast Level for pH, Titratable Acidity, and Sour Intensity with LSD Letter Codes to Indicate Significantly Different Groups

	light roast	medium roast	dark roast
mean pH	4.93 c	5.01 b	5.14 a
mean TA in mL NaOH	6.23 a	5.68 b	4.89 c
mean sour intensity	37.54 a	31.77 b	27.65 c

2.1.2. Temperature Experiment. A single medium roast wet processed Arabica coffee was used, comprising a mixture of Bourbon, Catuai, Caturra, Lempira, Ihcafe 90, Pacas, and Typica varietals from Honduras. The green coffee was mixed then roasted in a Loring S35 to a medium roast level, most similar to the medium roast in the prior roast experiment (2.1.1.). For full roasting parameters see Batali et al.[21] All roasting was performed on the same day, and batches were combined and well mixed postroasting to control for any variation among roasts. One week after roasting to allow off-gassing, coffees were packaged in 1 kg vacuum sealed plastic bags and stored in a −20 °C freezer. The nine TDS-PE combinations were brewed at three temperatures (87 °C, 90 °C, and 93 °C), adjusting the grind size and water pulsing duty cycle as needed to obtain the target TDS and PE values for 27 sample types total. With replication and multiple tasting sessions to accommodate panelist schedules, 270 individual brews were evaluated.

2.1.3. Consumer Experiment. The same coffee and brew settings used in the temperature experiment (Section 2.1.2) were evaluated by untrained consumers in single sessions over the course of three weekends.[23] Consumers evaluated each of the 27 distinct brews once. A total of 118 Northern Californian consumers were split into 8 different groups to taste 3 times for a total of 216 individual brews evaluated.

2.2. Sensory Analysis. *2.2.1. Descriptive Analysis.* Coffees in both the roast experiment and the temperature experiment were analyzed using a hybrid of QDA and Spectrum methods.[29] All work with human subjects was reviewed and approved by the UC Davis Institutional Review Board (IRB# 1082568). Volunteer panelists were recruited and screened based on interest, availability, previous experience with descriptive analysis panels, and correct completion of discrimination tests with coffee. The panel for the roast level experiment consisted of 12 judges, 9 women and 3 men, between 18 and 28 years of age. The panel for the temperature experiment was comprised of 12 judges, 8 women and 4 men, between 18 and 30 years of age. Panelists were trained on multiple attributes as outlined before.[20,21]

In both cases, panelists completed 14 tasting sessions where 6 coffees were evaluated per session. Evaluations were performed in temperature-controlled, red-lit sensory booths, where panelists were isolated. Samples were coded with a 3-digit random code and served in a randomized Williams Latin Square block design to control for carry over effects. Panelists evaluated all coffees in triplicate on separate days. Coffee was served in white ceramic mugs, filled with 50 mL of coffee, and then allowed to cool to 65 °C to control temperature for all panelists and serve at a safe and desirable consumption temperature.[30] Coffees were presented one at a time to panelists with a 2 min rest between coffees. All panelists were provided with unsalted saltine crackers, water, and an empty cup to expectorate.

The panelists assessed 32 different sensory attributes, many of which yielded statistically significant differences with respect to brewing conditions. Herein, we focus only on sourness, which invariably exhibited the largest changes in magnitude with respect to brewing conditions.

2.2.2. Consumer Preference Testing. Regular consumers of black coffee ($n = 118$) tasted 27 coffees that varied in TDS, PE, and brewing

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temperature over the course of 3 weeks. For each coffee, consumers rated overall liking using the 9-point hedonic scale (9 = Like Extremely, 5 = Neither Like nor Dislike, 1 = Dislike Extremely); the adequacy of consumption temperature, flavor intensity, acidity and mouthfeel using just-about-right (JAR) scales (5-point bipolar scale including “Too much,” “Too little” and “Just-about-right” options); and were able to describe the flavor/mouthfeel of the coffee by selecting terms from a check-all-that-apply (CATA) list of 17 attributes that were adapted from the relevant flavor descriptors as determined by the DA panel. All coffees were presented in a randomized sequential monadic fashion in 4 oz paper hot cups (Solo Cup Co., Highland Park, IL, U.S.A.) and labeled with three-digit blinding codes. Further details of study methodology are outlined by Cotter et al.[23]

2.3. Physical and Chemical Measurements. *2.3.1. TDS and PE.* Immediately after each drip brew was complete, the brew mass was determined by weighing the full carafe post brewing and calculating the difference with the empty carafe. After weighing the mass, an approximately 125 mL aliquot of coffee was removed and allowed to cool to room temperature. The TDS was measured using a digital refractometer, calibrated with room temperature deionized water. The laboratory refractometer was shown in previous calibration experiments to yield excellent agreement with oven drying measurements.[19] The PE was then calculated using the following equation derived from mass conservation arguments[15]

$$\mathrm{PE} = \mathrm{TDS} \times \frac{M_{\mathrm{brew}}}{M_{\mathrm{grounds}}} \tag{1}$$

The TDS, PE, and brew mass were measured for all 744 individual brews assessed over the three studies.

2.3.2. pH and Titratable Acidity Measurements. For all 744 brews, the remainder of the 125 mL room-temperature coffee sample after measuring the TDS was used to measure pH and titratable acidity. For pH measurements, 50 mL samples were delivered using a volumetric pipet into a 100 mL beaker with a stir bar. The pH measurements were taken of the sample while stirred using a Mettler Toledo S220 SevenCompact Benchtop pH/ISE Meter.

Titratable acidity was then measured by adding 0.1 M NaOH dropwise from a buret while the 50 mL sample of coffee was stirred, until reaching a pH of 8.2 ± 0.05. Titratable acidity is expressed here in mL NaOH/50 mL coffee. The pH meter was calibrated using acidic (VWR chemicals, pH 4.00 ± 0.01, color coded red), neutral (VWR chemicals, pH 7.00 ± 0.01, color coded yellow), and basic (VWR chemicals, pH 12.00 ± 0.01, color coded blue) calibration standards before every set of six measurements.

The pH and TA measurements were performed after the tasting session had ended, approximately 1 h after brewing. For the roast and temperature experiments, six samples were evaluated per session; therefore, pH and titratable acidity measurements were acquired in sets of six. There were three trial replicates for each panelist, but panelists were split into three groups due to testing facility capacity; measurements were taken at every individual tasting session, so there were 9 trial replicates for pH and TA measurements of the 27 TDS-PE-Roast or TDS-PE-Temp combinations. For the consumer experiment, there were no trial replicates for sensory evaluation (i.e., each consumer tasted each coffee once), but measurements were taken at every individual tasting session, so there were eight replicates of the TA and pH measurements for each sample. In the consumer experiment, nine samples were evaluated per session, so the pH and TA measurements were taken in sets of nine. In total, pH and TA data were obtained for all 744 unique drip brews.

2.4. Data and Statistical Analysis. *2.4.1. Roast Experiment and Temperature Experiment.* Descriptive analysis results were exported from RedJade, converting positions on 15 cm unmarked line scale to scores from 0 to 100. The measured TDS, PE, TA, pH, and sour taste intensity values were all averaged for each trial replicate for correlation calculations to give 81 data points per experiment.

Statistical analyses were performed using R version 3.5.1 (R Core Team 2020). Pearson correlation coefficients were calculated using the “ggscatter” function from the “ggpubr” package to both visualize data and calculate correlations. The function “ggscatter” was used to plot the data and calculate the Pearson correlation coefficient with α = 0.05, and the 95% confidence interval. Correlations between physical measurements were performed using raw data. Perceived sourness values represent the average score across all panelists in each replicate, and the pH and titratable acidity values were the exact measurements from each tasting session.

Response Surface Methodology[31] was performed using the “rsm” package in R to visualize how all sourness data from both descriptive analysis experiments related to TDS and PE. The same method was applied to TA data from both descriptive analysis experiments, to relate TDS and PE to the TA across all roasts and brew temperatures. Data was combined for both the roast and temperature experiment and calculations were performed with measured TDS and PE values to account for between-brew variation when mapping the dependent variables with exact values of TDS and PE and standard deviation shown by Frost et al.[20] and Batali et al.[21] Response surface maps for TA were also separated by roast level. PE and TDS levels were coded to −1, 0, and 1 (eqs 2 and 3), and the mean response intensity for each sensory attribute was averaged over all sensory replicates. Regression analysis was performed with a polynomial model shown for the first order fit in eq 4, and the second order fit in eq 5, as a function for the predicted response $E(Y)$ with β_0 as a constant, and β_1, β_2, β_{12}, β_{11}, and β_{22} as regression coefficients. x_1 and x_2 are the coded independent brewing control chart variables of PE and TDS, respectively.

$$x_1 = \frac{\mathrm{PE} - 20}{4} \tag{2}$$

$$x_2 = \frac{\mathrm{TDS} - 1.25}{0.25} \tag{3}$$

$$\text{First order: } E(Y) = \beta_0 + \beta_1 x_1 + \beta_2 x_2 \tag{4}$$

$$\text{Second order: } E(Y) = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{12} x_1 x_2 + \beta_{11} x_1^2 + \beta_{22} x_2^2 \tag{5}$$

Fisher’s F statistic and lack of fit were evaluated to determine model fit, beginning with first order fit and then applying second order fit only where necessary.[31] If any second order term was significant, the full model was retained.

2.4.2. Consumer Experiment. Three different analyses were conducted on the data generated from the consumer acceptance test. First, logistic regression models were used to relate the selection rate of the term “sour” in the CATA list to the TA and pH of the coffees, considering the entire consumer population. Logistic regression is necessary for this analysis because the dependent variable is a proportion (i.e., the proportion of consumers who selected a particular attribute) rather than a response rated on a continuous or interval scale such as intensities measured in DA. For the next two analyses, two consumer preference clusters are considered due to the presence of a significant Consumer*TDS interaction in the ANOVA for the 9-point hedonic scale responses. Preference cluster 1 (n = 51) displayed a higher liking for high TDS (>1.3) coffees and a lower liking for moderate PE coffees. Preference cluster 2 (n = 67) tended to like low TDS (<1.25) and low-to-moderate PE. Because of these divergent preferences, all JAR responses were broken down by cluster to investigate how these groups differed in their responses to the JAR attributes. Logistic regression models were constructed to relate the two chemical measures of interest to the selection rates of “too much acidity” and “too little acidity” (see Table 2). The general formula for the logistic regression models is provided in eq 6, where p is the proportion of affirmative responses (for a given TA or pH), β_0 is the centered intercept, β_1 is the regression coefficient, and x_1 is the standardized linear predictor (either TA or pH)

$$\log \frac{p}{1-p} = \beta_0 + \beta_1 x_1 \tag{6}$$

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The significance of logistic regression is defined by whether or not the confidence interval of the slope includes zero (Table 2).

Finally, penalty analysis was conducted for the acidity JAR following methodology described in the ASTM protocol.[32] Briefly, hedonic scores were separated into three groups based on responses to the JAR question (too much, JAR, too little). Mean overall liking scores were calculated for each group. Penalty was calculated by taking the differences between the mean of the JAR group and the means of the "too much" and "too little" groups. These differences are plotted against the proportion of consumers who selected either "too much" or "too little" and are again broken down by preference cluster. Here we only consider the results of the acidity JAR question; full details on other JAR questions can be found in Cotter et al.[23]

3. RESULTS

3.1. Variation in pH and TA with Brewing Metrics.

Focusing first on the pH, we find that the pH was only weakly correlated to TDS for light, medium, and dark roast coffee (Figure 2A). For the roast experiment, there was a slight negative correlation, indicating that as the TDS increases, the brewed coffee becomes more acidic, but this change was relatively small. For medium roast coffee, the pH decreased from approximately 5.0 to 4.95 for TDS values ranging from 0.8 to 1.6%. In other words, doubling the strength of the brew had almost no impact on the pH. Likewise, the light roast varied from pH 4.90 to 4.85 over a similar range of TDS, while the dark roast varied from pH 5.2 to 5.1. Although the correlations in each case were statistically significant ($p < 0.05$), the regression coefficients were small ($R = -0.22$ to -0.36) indicating only weak negative correlations. Even less variation in pH was observed with medium roast prepared at different brew temperatures (Figure 2B), where the pH exhibited no statistically significant variation from around pH 4.9 with respect to TDS or PE for any brew temperature.

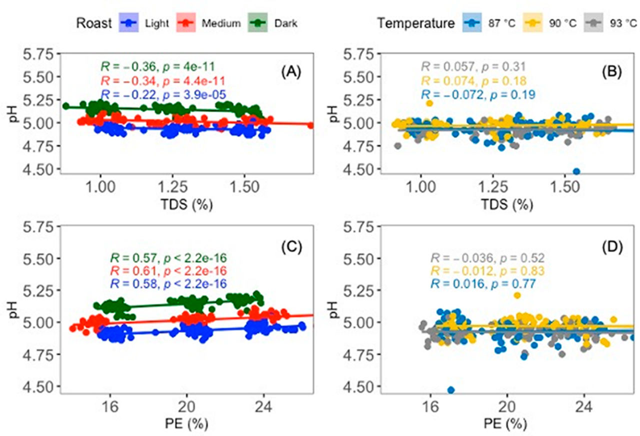

Figure 2. Correlations between pH and extraction measurements. (A) pH versus TDS, three roast levels, (B) pH versus TDS, three brewing temperatures, (C) pH versus PE, three roast levels, and (D) pH versus PE, three brewing temperatures.

With regards to PE (Figure 2C), all roast levels showed a significant positive correlation between pH and PE with all roast levels increasing in pH (i.e., becoming more basic) as PE increased. The magnitude of change was similar to the change observed with respect to TDS, varying from approximately pH 4.9 to 5.1 over PE values ranging from 16 to 24% for medium roast. Finally, just like with TDS the medium roast coffee at three different brew temperatures showed no correlation between pH and percent extraction. Roast does have a significant effect on pH with light roast the most acidic with a mean pH of 4.93 regardless of TDS or PE, and then medium roast slightly less acidic with a mean of 5.01, and dark roast the least acidic at 5.14. The overarching trend is that the pH varied little with respect to widely varying brew strengths and extractions yields.

In contrast to the weak correlations observed with pH, we found an extremely strong positive correlation between TA and TDS (Figure 3). For all roast levels and brew temperatures examined, the TA had a significant positive linear correlation with TDS (Figure 3A,B), with R values between 0.75 and 0.97. The titratable acidity doubled from approximately 4 mL NaOH/50 mL coffee to 8 mL NaOH/50 mL coffee in response to the TDS doubling from 0.8 to 1.6%. With different roast levels, there was a small difference between titratable acidity at equal TDS, but the separation is not as clear as it was for pH (cf. Figure 2A). The overall mean TA for light roast was 6.23 mL NaOH, medium roast was 5.68 mL NaOH, and dark roast was 4.89 mL NaOH. There was no difference in titratable acidity among brew temperatures at equivalent TDS (Figure 3B).

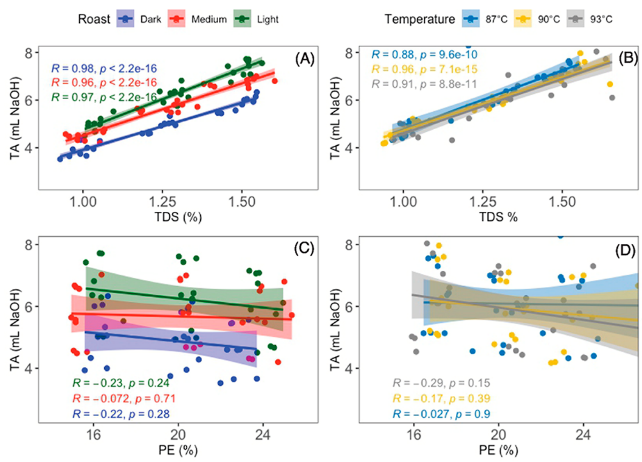

Figure 3. Correlations between titratable acidity and extraction measurements. (A) TA versus TDS, three roast levels, (B) TA versus TDS, three brewing temperatures, (C) TA versus PE, three roast levels, and (D) TA versus PE, three brewing temperatures.

In comparison to the strong linear correlations with TDS, the titratable acidity was only weakly correlated or uncorrelated with PE (Figure 3C,D). The light and dark roasts (Figure 3C) and 87 °C (Figure 3D) exhibited a very slight statistically significant negative correlation ($R = -0.21$ and -0.22), but only decreasing by about 1 mL NaOH as PE increased from 15% to 25%. The medium roast in the roast experiment exhibited no statistically significant correlation. In the temperature experiment, there was a weak negative correlation ($R = -0.24$) between PE and TA for the 93 °C brewing temperature, but a weak positive correlation ($R = 0.14$) between PE and TA for the 87 °C brewing temperature. No statistically significant relationship was seen between TA and PE at a brew temperature of 90 °C. Overall, Figure 3 indicates that the TA varies strongly with TDS but weakly at best with PE.

3.2. Relationship between Acidity and Perceived Sourness.

Turning now to sensory assessments by trained panelists, comparisons of the chemical measures to the

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descriptive panel results indicate that perceived sourness scores were negatively correlated with pH at all three roast levels (Figure 4A) with a higher, more basic pH perceived as less

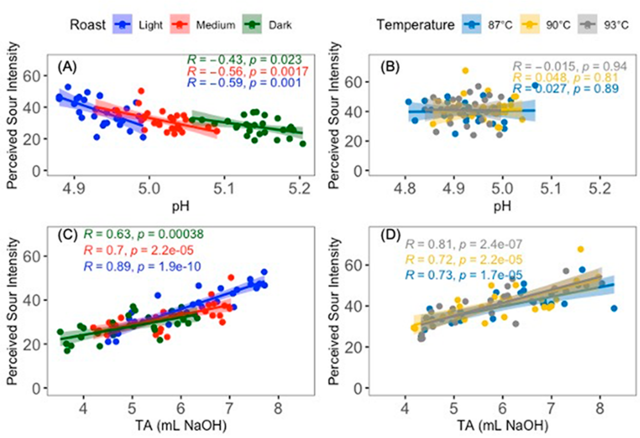

Figure 4. Relationship between chemical measures to perceived sour intensity by sensory panel. (A) Sourness versus pH, three roast levels, (B) sourness versus pH, three brew temperatures, (C) sourness versus TA, three roast levels, and (D) sourness versus TA, three brewing temperatures.

sour. There is some separation by roast with the range of perceived sourness slightly larger for light roast than dark roast but notably there is much overlap between roasts, different roast levels can readily be brewed to equivalent pH and sour intensity. Interestingly, there was no statistically significant relationship between pH and sourness intensity for the medium roast brewed at three different brewing temperatures (Figure 4B).

When examining the relationship between titratable acidity and perceived sourness (Figure 4C,D), we find clear positive correlations. Significant correlations were found for all roast levels, and interestingly, there was overlap in acidity and sourness across different roast levels depending on brewing (i.e., a low PE, high TDS dark roast can be just as acidic as a higher PE, lower TDS medium roast) despite the general belief that lighter roasts will be universally more acidic than darker roasts. The medium roast coffee from the temperature project also had a strong correlation between titratable acidity and perceived sourness (Figure 4D) but no difference in acidity or perceived sourness by brewing temperature.

3.3. Relationship between Sour Taste, Acidity, and the Coffee Brewing Control Chart. To relate more directly to the Coffee Brewing Control Chart inspiring this work, we can use response surface methodology to map perceived sourness and TA versus brew strength and extraction yield. The contour plots in Figure 5 model the relationship between sour taste (Figure 5A) or titratable acidity (Figure 5B) versus TDS and PE averaged over all coffees tested for both the roast and temperature experiments previously published individually.[20,21] Perceived sour taste has a strong relationship with both TDS and PE (Figure 5A) with coffees brewed at a high TDS, low PE being the most perceptibly sour. This follows a first order planar fit with the lowest sourness in the low TDS, high PE samples. Note that nonaveraged RSMs of perceived sourness for individual roast levels and brew temperatures are available in the prior studies, all of which exhibited qualitatively similar trends. We emphasize the RSM in Figure 5A is a

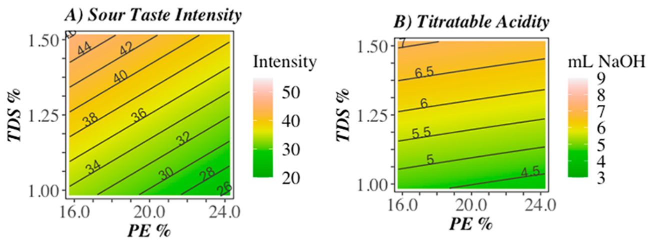

Figure 5. Contour plots of fitted response surface for (A) sour intensity versus total dissolved solids and percent extraction and (B) titratable acidity versus total dissolved solids and percent extraction.

"universal" depiction of sourness averaged over widely disparate coffees.

Contour plots of the titratable acidity reveal key differences in the relationship with TDS and PE compared to perceived sourness. First, the fit is second order, although the curvature of the second order fit is slight and difficult to see. More importantly, there was a much stronger relationship between titratable acidity and TDS than titratable acidity and PE, as the linear regressions in Figures 2 and 3 showed. Visually, this difference manifests in the very different slopes of the contour lines between the sourness RSM and the TA RSM; in the sourness map, sourness changes dramatically with PE (as indicated by the diagonal contours) but in the TA map, the TA changes only weakly with PE (as indicated by the much more horizontal contours). This result is significant because two brews can have the same TA and very different sourness. However, because titratable acidity actually follows a second order quadratic fit, there is a subtle increase in the relationship between titratable acidity and PE as PE increases. Thus, titratable acidity and PE may have a nonlinear relationship that is significant at higher extraction only. This nonlinear relationship was seen consistently in all roast levels (c.f. Supplemental Figure 1) with only a change in the magnitude of the data at different roasts.

3.4. Relationship between Acidity and Consumer Liking. Finally, we consider how untrained consumers assessed acidity versus brewing conditions. The rates of CATA selections for "sour" as a function of TA and pH are shown in Figure 6. Overall, the consumer test data showed a very clear increase in the selections of the term "sour" as a function of TA and a slight but consistent decrease in "sour" selections as a function of pH: the proportion selecting sour doubled from 24% of participants at TA = 4 mL NaOH to 50% of participants at TA = 8 mL NaOH.

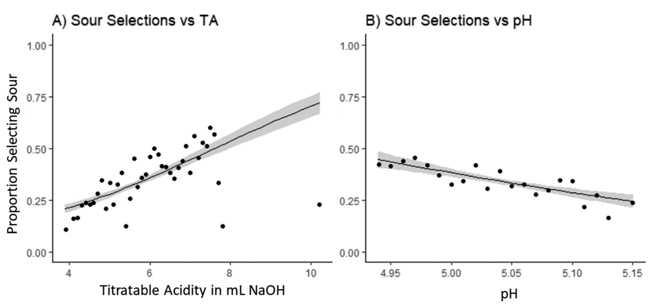

Figure 6. Logistic regression models of showing the proportion of consumers selecting the "sour" descriptor in the check-all-that apply list versus (A) TA and (B) pH.

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A breakdown of the responses to the acidity JAR question as a function of chemical measures of acidity (Figure 7) shows an increase in proportion citing too much acidity as titratable acidity increases. The proportion increased from approximately 10% to over 50% as the TA doubles (Figure 7A). Likewise, the proportion selecting too much acidity decreased with pH (Figure 7B). Selections of too little acidity (Figure 7C) had essentially opposite trends. Table 2 shows the slopes, intercepts, and confidence intervals for these figures. The consumer study broke down the results into two distinct clusters based on liking patterns, and although there were multiple drivers of difference qualitatively the two clusters can be characterized as Cluster 2, who preferred low TDS coffee, and Cluster 1, who preferred low and high PE coffee. Sour liking did separate the clusters with Cluster 1 generally being more of a sour-liking cluster. Cluster 1 selected "too little acidity" more frequently than Cluster 2, and "too little acidity" had a higher penalty on overall liking in Cluster 1 while "too much acidity" had a lower penalty. Cluster 1 had a much higher response rate of "too little acidity" than Cluster 2, especially at the lowest values of TA with nearly twice the proportion of selecting "too little acidity". Increase in pH offers mixed results in increasing the selection of "too little acidity" with Cluster 2 selecting too little acidity more often at higher pH whereas the responses from Cluster 1 remained relatively flat.

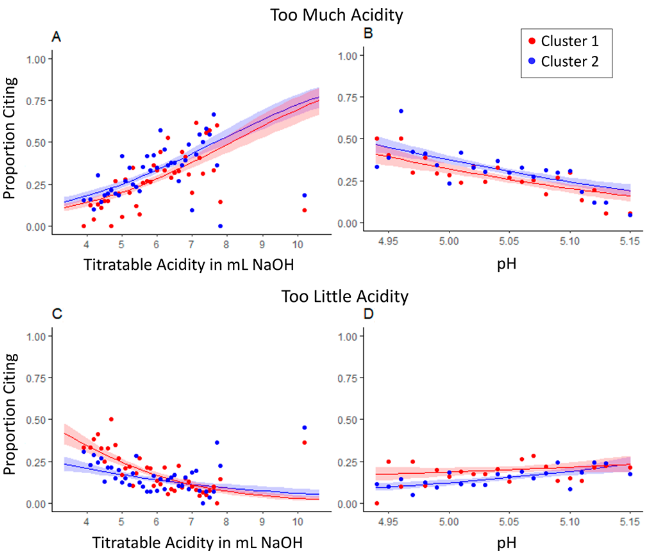

Figure 7. Logistic regression models of consumer test data relating JAR response rates of (A) too much acidity to TA, (B) too much acidity to pH, (C) too little acidity to TA, and (D) too little acidity to pH.

Table 2. Intercepts, Slopes, and Confidence Intervals for All Regression Analysis of the Consumer Data, Separated by Cluster

model	cluster	intercept	slope	.95% CI (slope)
too much acidity versus TA	cluster 1	−0.93	0.59	0.44−0.73
	cluster 2	−0.63	0.55	0.42−0.67
too much acidity versus pH	cluster 1	−1.00	−0.39	(−0.56)−(−0.22)
	cluster 2	−0.77	−0.39	(−0.51)−(−0.28)
too little acidity versus TA	cluster 1	−1.63	−0.65	(−0.83)−(−0.47)
	cluster 2	−1.84	−0.32	(−0.49)−(−0.16)
too little acidity versus pH	cluster 1	−1.41	0.12	(−0.07)−0.30
	cluster 2	−1.77	0.33	0.15−0.52
sour versus TA		−0.58	0.48	0.39−0.57
sour versus pH		−0.66	−0.28	(−0.38)−(−0.17)

Penalty analysis in Figure 8 visualizes how deviations from JAR acidity impacted the overall liking for the coffees for each of these consumer clusters. Regarding "too much acidity", it is again seen that Cluster 2 selected this to describe the coffees more often than Cluster 1 (32% versus 27%) and that "too much acidity" resulted in a higher hedonic penalty for Cluster 2 (1.5/9.0) than Cluster 1 (1.2/9.0). "Too little acidity" was selected less often overall than "too much acidity," however Cluster 1 selected this option more often (20%) and was associated with a higher hedonic penalty (1.8/9.0) than Cluster 2 (15%, 1.2/9.0).

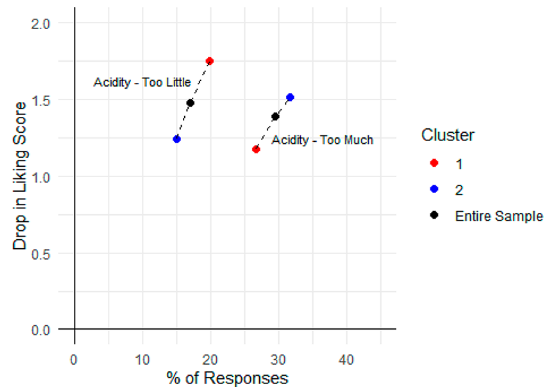

Figure 8. Penalty analysis showing the average drop in liking score associated with consumers rating a coffee as having either "too much" or "too little" acidity versus the overall percentages of responses for each consumer preference cluster.

4. DISCUSSION

4.1. pH as an Index for Sourness. Overall, our results show that sourness intensity as measured by descriptive analysis was correlated with pH only weakly. For the roast experiment, at multiple roast levels the sourness showed a weak correlation with pH, and high TDS, low PE coffee had the lowest pH and highest sour intensity. However, from our results we cannot confidently claim that pH is a good predictor, because the relationship observed in the roast does not necessarily hold true for all coffees. The medium roast coffee in the temperature experiment did not exhibit a statistically significant relationship between TDS or PE and pH, and the same experiment has no statistically significant relationship between pH and sourness. The inconsistency between the roast experiment and the temperature experiment could have been due to panel sensitivity with the roast panel slightly better trained to recognize small differences in sourness that would capture the trends with pH. Interestingly, there was a significant inverse relationship between pH and consumer selection of the term "sour" from the CATA list (Figure 6B), presumably indicative of sourness intensity. The consumer selections, however, are not an exact measure of intensity, which simply indicates that low pH coffee is more likely to give the impression of sourness to the untrained taster, but the average difference might not be at a high enough magnitude to show trends in intensity in all coffee types. Ultimately, there

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was more clear separation in pH among roasts than among brews. The results suggest that pH should only be used to predict sourness of coffee when comparing multiple roast levels at the same TDS and PE.

4.2. Titratable Acidity as an Index for Sourness. In contrast to the pH, our results show a clear linear correlation between titratable acidity and perceived sourness in drip brew coffee (Figure 3C,D). These results are chemically plausible because pH is a measurement of the dissociated hydrogen ion concentration, whereas titratable acidity is a measurement of acidic protons. Titratable acidity, therefore, should be a more accurate measure of the type of acids in coffee, organic acids which do not dissociate fully but still contribute to sour taste, as well as other sensory qualities such as bitterness,[6,8,10,13] astringency,[6,7,9,10,12] and aromas.[9,10] Our work here establishes that when evaluating relative qualities of different brewed coffees at different positions of TDS and PE on the Coffee Brewing Control Chart titratable acidity could be a useful index for predicting a sensory profile just as TDS and PE might. Furthermore, because titratable acidity increases linearly with TDS and correlates with perceived sourness (Figures 2 and 3), our results indicate that the TDS is an excellent proxy for the titratable acidity. Additionally, titratable acidity correlated with consumer perception of sourness as evaluated by CATA (Figure 6A). Compared to pH, titratable acidity is a consistent predictor of perceptible sourness shown in multiple and different roasts and brew temperatures. The correlation also holds true regardless of the evaluator: titratable acidity predicted sour perception by both trained expert panelists and untrained coffee consumers.

Our results also show that there are confounding factors beyond titratable acidity that will impact sourness, which explains previous literature questioning the adequacy of titratable acidity measurements for assessing perceived sourness.[7,33−35] Not all acidic compounds substantially contribute to sourness, or do not contribute to sourness at the same intensity, as is the case for caffeic and chlorogenic acids[7,8] compared to acetic and citric acids. Chlorogenic acids might be the reason for consistent titratable acidity despite lower sourness at high PE; Ludwig et al. showed that chlorogenic acids tended to take a longer time to extract than some other measured compounds in coffee[35] and thus might increase at higher PE. Additionally, the variation in other compounds in coffee could impact sourness perception despite similar measured acidity. There have been studies that have shown both the additive and suppressive combinations of bitter and sour tastes,[36] and varying extraction of bitterants could change perceived sourness at equivalent titratable acidity. Additionally, Bartoshuk et al. showed that binary mixtures of sour compounds would actually be less perceptibly sour than the sums of their individual intensities.[34] Ultimately, there are a variety of factors that may confound the relationship between TDS, titratable acidity, and perceived sourness, but it seems that in this more systematic study where fewer variables were changed there are clear relationships between TDS, titratable acidity, and perceived sourness. These results offer us another tool to predict a key feature of the quality of coffee beverages based on simple and measurable physiochemical properties.

4.3. Acidity by Roast. Unsurprisingly, both pH and titratable acidity showed differences by roast. It is well established that coffee progressively becomes less acidic as roasts progress, that is, green coffee beans have a high concentration of acids, which react, break down, and volatilize during roasting. Chlorogenic acids in green coffee will form chlorogenic acid lactones but will also break down to caffeic acid, quinic acid, and further into volatile acids and aromas.[37] Citric, malic, and other organic acids are formed during coffee processing but will degrade over the course of a roast and decrease overall acidity.[6] Volatile acids, like acetic and formic, will be driven off by heat during roasting and as such a darker roast would have a lower concentration of volatile acids as well.[38] Ultimately, it is well accepted that light roasts are more sour and acidic than dark roasts.

Interestingly, the results here show that for titratable acidity and perceived sourness, brewing can make nearly as much of a difference as roast. Although the average titratable acidity and sourness for light roast coffee was higher than medium and dark roast (Table 1), the overlap in the scatter of both TA (Figure 3A) and sourness scores (Figure 4A) indicates that coffees at different roast levels can be brewed to equivalent acidity. A high TDS dark roast can have a titratable acidity equivalent to a low TDS light roast. Note that though titratable acidity heavily overlaps between roasts, pH does not overlap nearly as much and is distinct to individual roast levels (Figure 2A,C)

It is clear in Figure 4a,c that despite the difference in means by roast there is substantial overlap in perceived sour intensity of all roasts. The roasts evaluated here were three different roast levels using the same green coffee, but with acidity being an important part of coffee quality[2] and sourness as a contributor to consumer liking[18] it is important to consider that differences in brewing can play a substantial role in manipulating that aspect of beverage sensory profile. In other words, a light roast coffee is not doomed to be overly sour or a dark roast to be dull and flat; judicious choices in brewing can yield a wide range of sourness in either roast level. Ultimately our results hint at tremendous flexibility to personal preference, that is, a consumer can have the flavor characteristic of a roast level they like while still controlling acidity and sourness to their personal preference through brewing.

4.4. Acidity by Brewing Temperature. The lack of difference in acidity by brewing temperature, in conjunction with our previously reported sensory results showing minimal sensory difference,[21,23] was surprising given common beliefs of the coffee industry. The Coffee Brewing Handbook published by the Specialty Coffee Associations states that "both acidity and body increase when the coffee is brewed at higher temperatures".[16] Controlling for extraction, Pangborn found that in a brewing range from 65°−100°, sourness, as well as bitterness, progressively increased.[39] Finally, in espresso coffee it was shown that espresso brewed at 98 °C was more sour than 88 °C, but the higher temperature coffee was higher in TDS,[40] which is consistent with our sensory results. At fixed TDS and PE, there is little to support the belief that higher temperature brings out more acidity; our chemical and sensory results indicate that TDS and PE control the titratable acidity and perceived sourness, not the brew temperature. The main role of the brew temperature is to affect the dynamics of extraction and thus alter the TDS and titratable acidity, which are the factors that actually determine sourness. There are many other factors, such as grind size, bed depth, brew time, and brew ratio that can impact the TDS and resulting acidity and sourness at equivalent brewing temperature.

An important caveat is that we only studied brew temperatures over the range 87 to 93 °C. The results presented here thus do not address claims that cold brew is

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less acidic. Experiments over a wider range of temperatures are necessary to investigate that hypothesis.

4.5. Acidity and Consumer Preference. Overall, even untrained consumers were generally able to tell the difference between low and high TA coffee with the proportion of consumers selecting sour on the CATA doubling as the TA doubled. Untrained consumers also noticed a difference with lower pH, selecting sour less frequently. Ultimately, these results indicate that the average consumer, not just expert panelists, will also potentially perceive differences in sourness based on brewing and resulting acidity. Changes in TA and pH also impact consumer liking, though the preference clusters indicate that acidity liking is not equal across all consumers. Overall, Cluster 1 was more likely to select "not enough acidity" and less likely to select "too much acidity" than Cluster 2. Cluster 1 was slightly smaller (n = 51) than Cluster 2 (n = 67), so the sour-liking cluster was in slight minority but they still made up a substantial portion of coffee consumers. As TA increases, overall selections of "too much acidity" increase, but it seems that a relevant portion of consumers might find the increase in acidity appealing. In previous coffee literature, Geel et al. also saw a smaller but notable cluster of consumers who were identified as preferring more acidic coffee.[41] However, when evaluating overall liking for unsegmented consumers, acidity or sourness scores have been shown to decrease overall consumer liking for cold and hot brew coffee.[18,42,43] The results here show that titratable acidity can be a predictor of whether consumers will perceive coffee as acidic or sour but that could be positive or negative depending on the consumer. Though the majority of consumers in most studies found sour coffee to negatively impact liking, the clusters that do find sourness more appealing are an important and valid portion of the consumer base. Unfortunately, neither Cotter et al. nor Geel et al. found any strong demographic correlations to how consumers prefer their coffee, and ultimately it would be valuable for the coffee industry to understand what kinds of consumers like what kinds of coffee to better understand how chemical measures of brews can predict customer liking.

4.6. Future Work. Our findings on titratable acidity, pH, and perceived sourness provide a foundation for understanding the chemical basis of sour perception, but coffee is a complex beverage and not all acids contribute to taste and/or aroma equally. Unanswered questions include the specific acid composition of brewed coffee at varying roasts and extraction levels to understand how specific compound extraction rates are impacted by brew method and how those compounds contribute to the sensory profile of coffee. For example, measuring antioxidant activity in coffee may give an estimate of chlorogenic acid concentration, which could in turn provide an estimate of nonsour tasting acids. In addition, the work presented here only applies to filtered drip brew hot coffee, but there are a multitude of other ways to brew coffee that deserve study. Cold brew coffee, for example, has been considered by the industry to be less acidic than hot brew, and literature has reported cold brewed coffee below 25 °C to be perceived as less acidic,[4,22,44,45] though not all of these studies were systematically controlled for TDS and PE. Additionally, espresso coffee is a vastly different high-pressure, fine-grind, high TDS brewing method, and acidity is important to espresso quality. Andueza et al. have suggested that pH is not an adequate predictor of perceived acidity in espresso.[46] In a study on pod espresso coffee, a decrease in pH and an increase in titratable acidity with extraction temperature found that coffee species played more of a role in the perception of acidity (i.e., Robusta blends) than the temperature and chemical measures of acidity.[47] Ultimately, most studies lack systematic characterization of extraction and chemical/sensory qualities only related to brewing parameters without confounding factors.

The research presented here provides a foundation for understanding how coffee acidity relates to strength and extraction (i.e., TDS and PE) as well as roast and brew temperature. We demonstrated that TDS and titratable acidity are linearly correlated and titratable acidity is in turn correlated with sourness. Coffee roasted to different levels can be brewed to the same acidity and perceived sourness depending on extraction, and higher brew temperature does not necessarily produce more acidic coffee. Furthermore, different consumers will have their preferences for coffee driven in part by the acidity they perceive. Understanding the relationship between titratable acidity and extraction offers another metric through which the coffee industry can predict the sensory profile of coffee, and alongside that our work provides further understanding into how brewing parameters impact sensory profile and acceptance.

ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available free of charge at https://pubs.acs.org/doi/10.1021/acsfoodscitech.0c00078.

Supplemental Figure 1 of response surface maps for titratable acidity of individual roast levels (light, medium, and dark) (PDF)

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