Matter

CellPress

Backstory

Chemistry and Coffee

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Chemists and Coffee Shops

On paper, I have had a privileged, short career in chemistry academia; I received an undergraduate degree from Monash University (2011) and a PhD from the University of Bath (2015), followed by a short postdoc at MIT. In 2017, I joined the University of Oregon and currently head an independent research group studying electronic structure of porous metal-organic scaffolds. However, I also have a side-gig in the coffee industry, which has been quite successful despite having no funding or time to work on these projects. This Backstory describes how this came to be.

My unusual career in coffee science began in 2014 on my commute up the hill to the University of Bath. Both my colleague, Alex Murray (now a lecturer at the University of Kent), and I would deliberately take a convoluted route to a less busy bus stop. This route also happened to pass our local cafe, Colonna and Smalls. Although we didn't realize it at the time, the café had evolved to become somewhat of a legendary shop; its owners, Maxwell and Lesley Colonna-Dashwood, had won the 2012 UK Barista Championship and ranked as a championship finalist at the World Barista Championship later that year. They take coffee seriously and think deeply about how to use flavor—an inherently subjective property—as the basis of their business.

At Colonna and Smalls, the menu is far more detailed than an average café. It is analogous to a wine list. Customers must choose a coffee and a format in which they would like to enjoy it (Figure 1). The menu provides information about the country of origin, the variety, the processing method (e.g., natural, pulped natural, washed), and, perhaps most importantly, the expected flavor notes when the coffee was consumed either as a filter, as an espresso, or an espresso paired with milk (e.g., a cappuccino, flat white, etc.). Despite being from Australia—a country that thinks very highly of their coffee—I had very little knowledge of the brown beverage. I was drawn to naturally processed coffees because they seemed to taste like blueberries, strawberries, and fortified wine. But perhaps the most impressive aspect of Colonna and Smalls was how Maxwell and Lesley could deliver extremely high volumes of information while simultaneously making the customer feel comfortable and excited to try the drink. I spent a lot of time in this cafe, and I learned a tremendous amount about how to communicate with people from vastly different backgrounds—this made me a much better scientist.

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In 2014, coffee science was viewed as a "hipster" alternative to the conventional third-wave coffee shop experience (i.e., shop's that present a coffee's terroir, create an environment for the customer to enjoy the beverage, and place a high value on personnel—the barista, the customer, the roaster, the producer). The third wave was riddled with cafes justifying how their drinks came to existence using patchy physics and chemistry. As scientists, we see this all the time. And this is not a criticism

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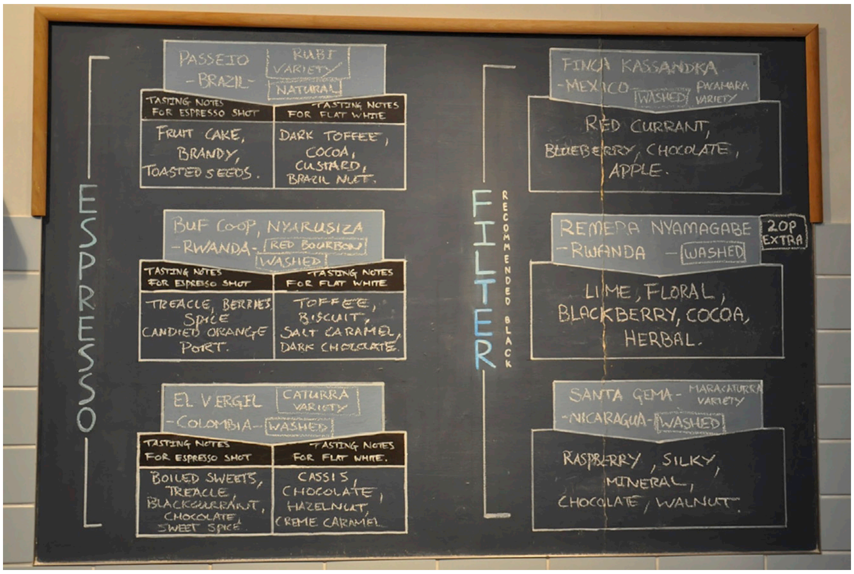

Figure 1. A Representative Menu at Colonna and Smalls, Bath, United Kingdom
Image reproduced with permission from Brian Williams, brian-coffee-spot.com.

of, or limited to, the coffee industry—coffee professionals know more about fundamental science than most of us know about coffee. The issue is simply one of communication; we need to share our knowledge with each other. Maxwell and Lesley were certainly not using coffee science as a selling point in their cafe; the flavors in their coffee spoke for themselves. The shop was more like an art gallery, but they were interested in how chemistry played a practical role in conveying these flavors.

While the industry as a whole continues to strive toward excellence in flavor and reproducibility, the scientific toolbox available to the barista is limited. For example, while the Specialty Coffee Association had developed recommendations for mineral compositions in brew water (long predating my interest in the subject), the document itself was overly prescriptive and didn't provide the average person with helpful insights beyond what was judiciously deemed "good" and "bad" water. Indeed, my first project in the coffee industry addressed this exact topic with the primary goal of improving scientific literacy, *not flavor* (that was secondary). A particular focus was placed on working with individuals who had no formal training in the natural sciences.

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The Transition from Curious Customer to Coffee Water Chemist

The menu at Colonna and Smalls changes every few days, making it one of the most exciting cafes to visit, and most challenging to operate. The coffees themselves are roasted all over the world, and only exceptional quality coffees are presented. My journey in coffee science began with one particular coffee that, no matter what brew method, brew ratio (mass-of-coffee to mass-of-water), grind setting, and water temperature, a persistent unpleasant flavor was detected in the cup. Upon consultation with the roaster, a reputable company located in London, it became clear that the water chemistry must be augmenting the flavor profile of this particular coffee. London has extremely hard and chlorine-rich tap water, which must be

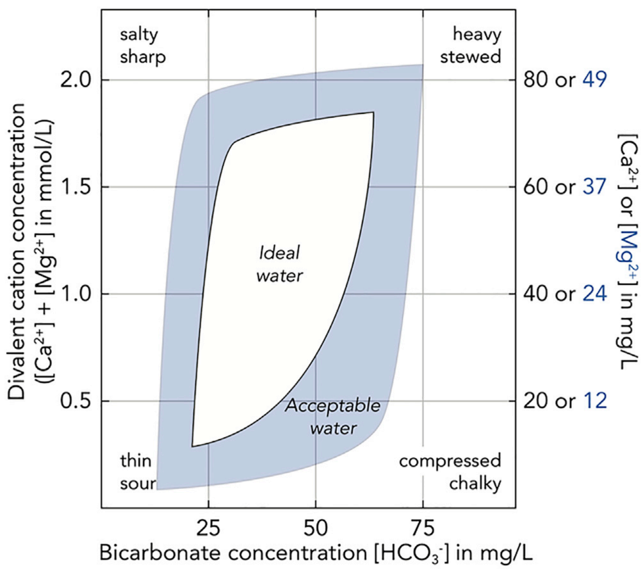

Figure 2. Recommended Water Chemistry for Brewing Balanced Cups of Coffee
Image adapted with permission from *Water For Coffee* (2015), Maxwell Colonna-Dashwood and Christopher H. Hendon.

reverse-osmosis treated to prevent limescale deposition and chlorine-catalyzed pitting corrosion. Bath also has hard water, but is unusually rich in sulfate (which is benign at < 250 mg/L) and, hence, only needed ion exchange to mitigate limescale deposition. Retrospectively, these were writ large chemical differences.

In 2014, however, the standard method for assessment of water composition was through a handheld ionic conductivity measurement. The obvious flaw in this measurement is the lack of qualitative information—are the ions all Na^+ and Cl^-? Perhaps the water contains more exotic chemistry? We later deduced that the primary reason the coffee was tasting different between two similarly conductive waters could be attributed to fluctuations in HCO_3^- content.

Coffee is inherently acidic, and HCO_3^- is efficient at stabilizing aqueous pH, thereby augmenting its perceived acidity. With this in mind, we developed an empirical water composition chart (Figure 2), which related the divalent cation concentration (thought to contribute to flavor extraction by controlling the ionic strength of the water; Hendon et al., J. Agric. Food Chem., *62*, 4947-4950) to the HCO_3^- composition (i.e., the buffer). The chart helped the community understand what solvated cations and anions were, and how they could impact the qualities of a cup of coffee. As a result, the coffee community shifted to performing in-cafe titrations using a procedure presented here (https://www.youtube.com/watch?v=2D5RTrSZQ7s). The success of this study was, in part, due to us *not identifying a unique* water composition that made tasty coffee, but rather a describing a range, outside of which yielded less desirable cup characteristics. After working together for over one year, Maxwell proposed that he used our work on water chemistry in his 2014 UK Barista Championship routine. At the time, I was unaware of the impact of the work, as well as the format and scale of the competition.

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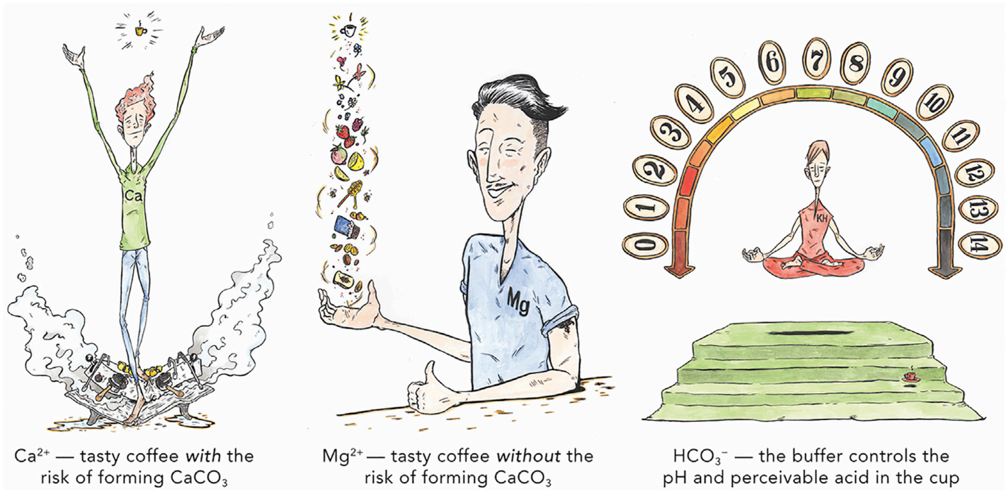

Figure 3. The Protagonists in Brewing Water Chemistry
Reproduced with permission from *Water For Coffee* (2015), Maxwell Colonna-Dashwood and Christopher H. Hendon; art by Peter Grosvenor-Attridge.

Competitive Coffee Competitions

The competition is essentially a choreographed production of 12 coffee drinks in 15 minutes. Four calibrated judges are presented drinks in waves: an espresso, a milk-based drink, and a signature beverage (e.g., espresso with added non-alcoholic ingredients; a classic example is the mocha). Judges also assess technical aspects of the routine (e.g., level tamping, consistent shot times, etc.) but one category reigns supreme—*flavor*. Maxwell presented all of our work on water chemistry by distilling the key concepts into three illustrated characters (Figure 3) and their impact of flavor. He went on to win the 2014 UK Championship and inevitably ranked 5th in the World Barista Championship in Rimini, Italy—his routine is worth watching (https://www.youtube.com/watch?v=VWax6Yr2oSU). We later self-published a book, *Water For Coffee*, which was essentially an applied general chemistry text for coffee professionals, although we stopped printing it in 2017 because there were some issues in some of my descriptions. For example, I used water as an example when describing the ideal gas equations. These things happen, and another edition will be published eventually.

Much like edition one of *Water For Coffee*, the competition is imperfect—the judges are humans, and humans have preferences. The machines have some variability between seemingly identical shots of espresso (the focus of our paper in this issue of *Matter*). The coffee is off-gassing and aging over the week of competition. The water chemistry at the competition is predictable, but vastly different to the water used in the testing at the roastery in preparation for the competition. But the competition is fun, and there is a lot of money at stake, so it continues to exist. In fact, Maxwell and I revisited the Barista Championship again in 2015, again somehow ranking 5th on the world stage later that year. In that routine, I helped Maxwell develop a signature drink, which was based on recreating the chemistry of a Pinot Noir (a banned substance) (this is discussed in more detail in Hendon, Science, *365*, 553). Between partnering with champion baristas, Maxwell and Lesley, writing *Water For Coffee* while also writing up my PhD thesis, and publishing open-access papers, my career in coffee was jump-started.

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Coffee Conferences

Since 2014, I have become a perennial speaker that the Specialty Coffee Association Expo. While the event is primarily a tradeshow, it also hosts the annual US Barista Championships and a series of lectures and workshops. The event is approximately the same size as the ACS National Meetings, but the coffee community is far more integrated: it doesn't matter whether you are a barista, CEO of an Italian company, a scientist, or a curious onlooker—you are welcome. The conference is literally delicious, the seminars are extremely well attended, and the social activities in the evenings are remarkable. I first presented on water chemistry in 2015, but somehow made it habitual to present new content each year. This may be why I continue to perform coffee research, knowing that I have a self-inflicted expectation to outdo myself at Expo. This year, it is conveniently held in Portland, OR, and it would appear that I have something to talk about!

Systematically Improving Espresso?

Three days before I left to start my postdoctoral studies in Boston, I borrowed a laser diffraction particle size analyzer and performed a series of experiments in the cafe. I wanted to address whether the grinder was turning coffee into equal sized dust, independent of the origin, processing method, and roaster (Uman et al., Sci. Rep., *6*, 24483). We needed these grinding data because they provided insights about the size of coffee particulates, which could be then fed into a model that could be used to predict extraction properties of espresso. Our initial goal was to optimize our grind settings so that we could be confident that the judges would enjoy four shots of identical espresso, and we could go and win the championship. But Maxwell retired from the competition, and I moved to the USA and got busier with metal-organic frameworks and surface catalysis, so the competition efforts were put on hold.

This project was restarted by Michael Cameron, a well-known barista whose work was well received in the coffee blog sector. We began working and communicating over Instagram—a social media platform infrequently used in academia, but widely used in coffee. His non-linear extraction data motivated Jamie Foster and me to adapt the model to understand the physical origin of this phenomenon. The paper spent another year on my desk because we knew this paper was going to get "peer-reviewed" by *a lot* of people in cafes. We needed to make sure all of the data were correctly interpreted and reproducible and the writing was terse but lucid so that both coffee professionals and scientists would appreciate its novelty. We think we managed it, yet somehow there is still more work to do. One thing is certain; if we cross paths at a conference, there is a good chance I can point you toward a tasty coffee shop nearby.

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