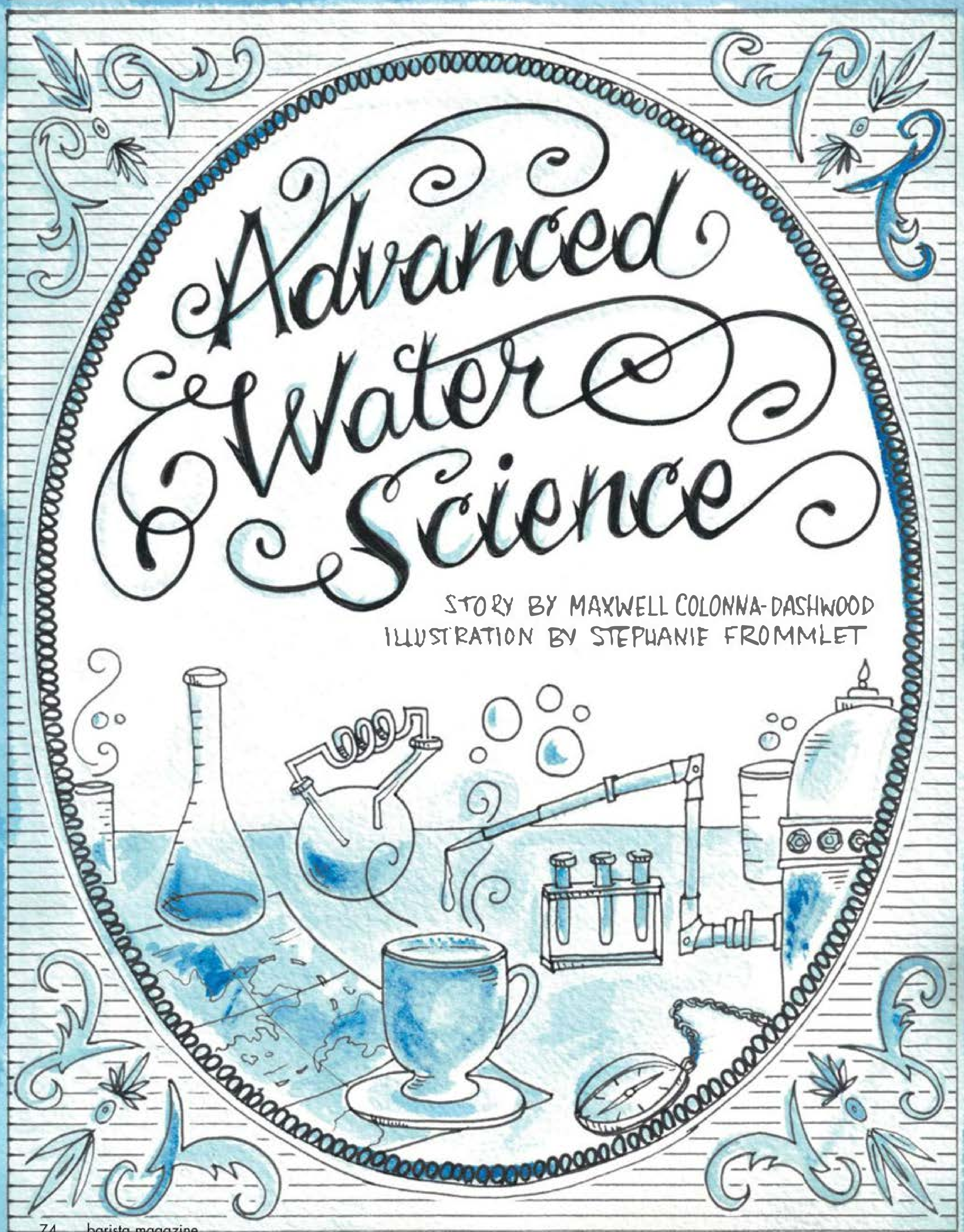
Advanced Water Science
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COFFEE IS AT ONCE both incredibly simple and intensely complex. On the one hand, it's a solution of water and a ground roasted seed. On the other hand, it is also varieties, processing, extraction percentages, moisture content, particle distribution, dense amounts of aromatic compounds, and so much more.

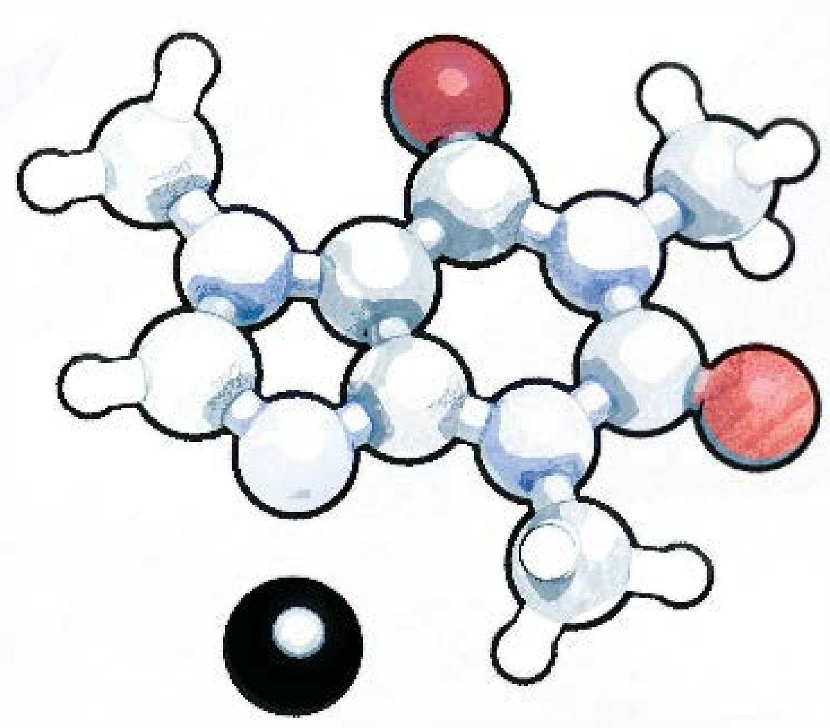
This is a fitting parallel for water. Water is a transparent, simple thirst-quencher. But it is also a complex solvent with buffering systems, a home to various compounds and all sorts of abilities which are at the core of our existence.

The importance of water in coffee has been well documented, but its particular and varied impact on the flavor of coffee has been less explicitly understood.

Just over a year-and-a-half ago, I was dialing in an espresso, trying to get a good balance of flavor, body, balance, and acidity.

I couldn't do it.

I tried everything—exploring extraction, brew strength, and all of the variables within our remit, even different grinders. No luck.



It tasted dull, heavy, sour, woody. It wasn't just a bit off; it was actively unpleasant. It's never nice to phone up a roaster and tell them their coffee doesn't taste very good. This was a such a rare thing to happen, in fact, that before I phoned them up, I double checked to make sure there was nothing I had missed. The roaster was naturally concerned and had a sample of that roast to test. After going away and experimenting with the coffee, he came back to me with a surprising result: It tasted fine when they brewed it.

Knowing each other's tasting background, it was safe to write off preference—this was something more fundamental. We chatted about each variable, referencing the grinder used, the recipe, and we touched briefly on water. We discussed TDS (total dissolved solids) as I'm sure most baristas have, which is measured by using a small conductivity meter with room-temperature water. We were around the recommended TDS, if slightly high, at 170ppm. We briefly ticked water off of the list, as well. But after repeated pondering of the problem, it quickly became apparent that this measurement couldn't be telling us the whole truth. The other variables just couldn't make it taste this bad. Questions quickly arose, such as, 170 parts of what?

Water was and is on the minds of many specialty-coffee professionals throughout the industry. After all, it's the ingredient a roaster can't really control. Reading everything I could find on water and coffee didn't really give me the answers I was looking for.

What to do?

Luck would have it that the close proximity of the University of Bath to the U.K. shop I own and operate with my wife, Colonna & Smalls, means that a collection of academics and scientists from various fields pass through our doors daily. This not only provides for interesting chitchat and a customer base with a natural inclination toward specialism, it also provides the opportunity to present questions that can draw on varied expertise, the potential being answers and investigations that approach coffee problems from very different angles.

Enter Christopher H. Hendon, a computational-theoretical scientist based in the chemistry department at the university. Chris is an outgoing, enthusiastic chemist (something of a rarity). He enjoys teaching chemistry and helping those of us without a deep knowledge of that world to understand its impact. Not only does he love using science to solve complex problems, but he likes applying that process to things we experience, especially food and drink.

He seemed like the right guy to present this water problem to. "Hey, Chris," I asked him. "This TDS reading, what does it really tell us about the water?" "Not that much," Chris replied. "Why do you ask?"

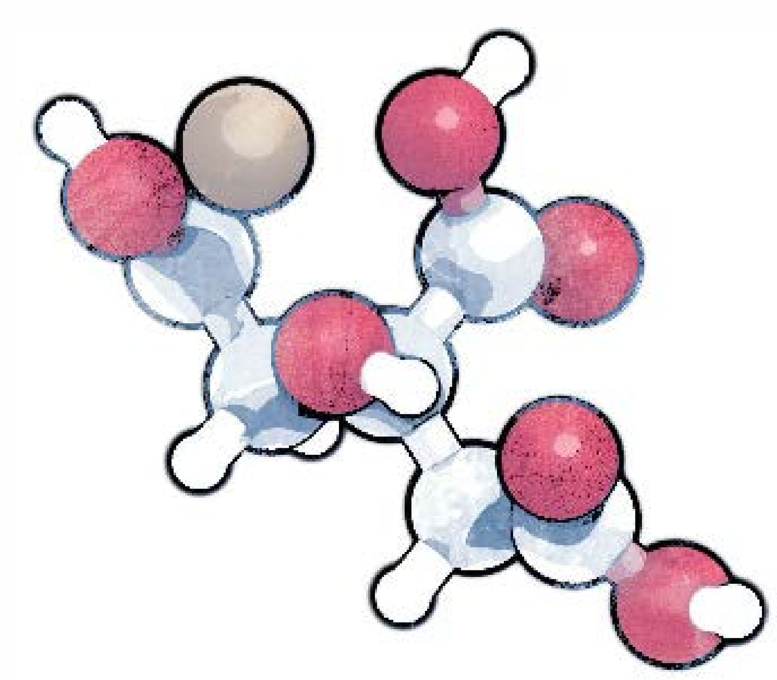
And so began a project and collaboration that has taken us to some really exciting places since that fateful day when my coffee tasted so mysteriously bad. We have even had a scientific paper on the subject published. [Editor's note: Maxwell's explorations into water science were the basis of his 2014 U.K. Barista Championship performance, which earned him the national title, and a rank of fifth at the World Barista Championship in Rimini, Italy, in June.]

Together, we approached the problem by looking at water chemistry first, and then at coffee. This was followed by the combination of the two. What do they mean to each other?

We discussed current water recommendations and the different reasonings exchanged within the coffee industry. This allowed us to focus on answering the right questions and write off the irrelevant and misleading inquiries.

Our first port of call was to look at the varying minerals in water and to discern the impact they may have on the coffee. With the help of a large and obscenely powerful supercomputer, we ran computational calculations to assess the different binding energy that the different minerals would have on different compounds in coffee. It is this aspect of our work that has been published in the *American Journal of Agricultural and Food Chemistry.*

It has long been documented that really soft water isn't able to pull enough flavor out of coffee, and here we were studying this process in detail. Binding energy is simply the mineral's likelihood of sticking to other compounds and pulling them into the brew. We could quickly eliminate many of the minerals from our realm of interest as they displayed low binding energy. In the case of something like sodium, the binding energy result was negligibly different to that of water itself. It would therefore take up numbers (within our TDS reading) without impacting on the extraction (in large quantities it will of course start to display itself independently as a taste).



This alone is a particularly interesting notion. It's easy to focus on the flavor of the water itself, surmising that the flavor of the water plus the flavor of the coffee equals the final beverage. This is a misleading and ultimately incorrect way to consider the two ingredients. Water is a solvent and a coffee bean a collection of complex organic compounds. When these two come together, we get a beverage that is unique to their combination, and the flavor of the water itself is lost. Eighty parts of magnesium, for example, is completely wiped out by the intense and comparatively huge amounts of coffee compounds that have entered the solution. It's therefore the magnesium (or other minerals) binding energy altering what's being extracted into the drink. This ability is far greater than their inherent flavor.

For the test, we picked several common compounds that are tasted in coffee, such as citric acid and quinic acid. The computational results showed that on all accounts, magnesium and calcium were the ones to watch. Magnesium displayed a higher overall pulling power than calcium, but calcium still showed significant pulling power in its own right.

It was interesting, however, to note that they had slight differences in preference. For example, the results for magnesium suggested that it would extract a slightly higher percentage of the brighter and fruity-tasting acids such as malic and citric, whereas calcium showed a slightly higher preference toward chlorogenic and quinic acid.

This would then suggest that coffee made with different ratios of magnesium and calcium, but to the same overall amount (TDS), would result in different tasting cups of coffee. However, there was a curious and substantial question to answer at this point. Most of the water concepts and theories I had heard previously stipulated that a higher TDS would saturate the water and leave no room for coffee extraction. The thing is though, if minerals increase extraction, would a high TDS really lower it? After all, a high TDS for coffee-brewing water is still a very dilute solution.

From a chemistry and physics point of view, this just doesn't hold up. You would need a TDS reading in excess of 1,000 parts per million to even begin to see this saturation issue. This confuses things further, though, as it means a high TDS water should create a full, flavorsome coffee—but it really doesn't. High TDS waters tend to produce dull, flat, and bitter brews with lowered acidity.

Conjugate partners: The evil twin.

Answering this question is really where our theory on water and coffee turned a corner and a cohesive concept took place.

To solve this problem, we needed to look at the role bicarbonate plays in the process. Bicarbonate is a base (alkaline) but it also acts as a buffering system for the water. So what's a buffering system? It's pretty damned cool, that's what.

Buffering systems in liquids are extremely important to a lot of things in a lot of ways. A good example of a buffering system is human blood, which needs to keep itself between 7.25 and 7.45 on the pH scale in order to keep us alive. It does this by managing the amount of compounds that are acidic and those that are alkaline. Let's take citric acid, for example. This is a weak acid. What this means is that it can easily be turned into a base/alkaline. It is still citric acid, but the proton has been knocked off and now it is something called a conjugate partner. I describe it as the evil twin of citric acid. This is not citric acid's natural state, but it's one that it can inhabit. Most compounds have this dual nature.

What does it mean for coffee? Well a lot of what we taste in coffee is acidic compounds. And we, of course, really value positive acidity in coffee (not all acids taste typically acidic, nor pleasantly acidic). A high buffer or bicarbonate content then acts as a buffer to try and neutralize the cup of coffee—but we don't want it to be neutralized. It doesn't have the same needs as our blood. In doing so, the buffer makes a lot of the pleasant tasting acids taste dull, flat, bitter and alkaline.

Hard waters tend to have a good amount of calcium and magnesium, but the bicarbonate content also tends to go up disproportionately, and a TDS meter doesn't tend to give a reading that is fully informative of the bicarbonate content. For example, you can have a water with a 300ppm TDS reading and a bicarbonate content in excess of that very total.

This means that a harder water will actually extract well or even in excess, but that the buffer will undo all of this and reverse a huge chunk of the flavor compounds. It then becomes apparent that a balance between the binding minerals and the bicarbonate is needed. This doesn't just explain hard water, it also explains why very soft water can result in empty, slightly sour brews. It turns out that we actually need some buffer to balance the acidity. Very soft waters or medium TDS (a certain TDS doesn't equal a certain bicarbonate content) waters with low buffer can result in quite sour and sharp brews.

There are then all sorts of water make-ups that will result in different results. You can pair magnesium and calcium (which are often measured as a combined total called "general hardness") against the buffer (often referred to as alkalinity or "temporary hardness") and ascertain the likely result. There is of course then a recommended sweet spot. It's exciting to test these theories out and find them ringing true in the cup.

Still much more to learn.

Chris and I are close to completing a water and coffee guidebook that chronicles our findings and acts as a user's manual. This book also includes a graph that charts these two numbers and the likely results in the hope of making the information as useful and accessible as possible. In the book, we also look at filtration systems and how they affect our water, moving beyond the simple goal of controlling TDS.

Other questions begin to arise in light of this knowledge. Are coffees being roasted to water? That is, in a soft water area will a coffee be roasted and brewed to tame the acidity that the water is unbalancing?

The questions and the potential answers are so fundamental to coffee and particularly pertinent for the world of speciality coffee.

We are excited by what we have been able to learn through the application of science to coffee, but feel there is so much more to explore. For water, we aim to tackle the same questions from different scientific angles. Our tests so far have revolved around the realm of theoretical chemistry. This means the creation of theories and models that are tested and validated with high-powered computers. Next is varied physical analysis to assess the compounds that are in the different coffees brewed with different waters.

An understanding of water's impact on coffee is vital to achieving consistently great coffee, and we hope this research can improve the dialogue within the specialty-coffee industry. Science, though, has a much more varied applicability to coffee. Scientific approach has been and is used in the coffee world, but the high costs and lack of accessibility mean that it's often employed in the more commoditized aspects of the coffee market, such as how to most efficiently extract 100 percent from the bean rather than 20. This research has traditionally been undertaken by big companies in the search to make the best margin from instant coffee.

It is exciting that the work we have done has attracted the interest of other scientists from different fields. Discussing the questions that we in the specialty-coffee industry have can often surprise the listener with the realization that specialty coffee is complex and that there is a lot to explore. This dawning realization of coffee's depth is commonplace for specialty coffee though, and not just within its scientific arm.

Upcoming projects include the separation of proteins in coffees using gels, followed by an assessment of protein breakdown in each. Hopefully there can be a correlation found between protein breakdown and desired roast levels. This technology originates from the study of disease and protein damage in our bodies, which we don't want. We do, however, need a certain amount of this degradation to occur in roasting, as many of the by-products are tasty. There also seems to be a fair bit of interest in grinding, with lessons from the pharmaceutical industry proving likely. Such experiments include air grinding and the assessment of something called surface disruption, where the surface of the coffee is altered when it's ground, but reverts to its original state due to the presence of humidity.

Who knows what the future holds for our understanding of coffee?

Science in coffee can seem aloof and exclusive, and it has often been suggested that coffee becomes too scientific. These, however, are broad brushstrokes of reason. Science is so varied; really it's about our application and use of it. It's about asking good questions, and for specialty coffee, it's about using science to increase our understanding of why and how coffee tastes the way it does so that we can more consistently make coffee that tastes great. With specialty-coffee science, it's all about flavor. b