LIGHTER

THAN AIR

WHAT AIR-QUALITY ENGINEERING CAN TELL US ABOUT COFFEE

by Jon Ferguson

Admittedly, the following words don't exactly roll off the tongue: Solid-phase microextraction (SPME) and multidimensional gas chromatography–mass spectrometry–olfactometry (mdGC-MS-O).

But these complex-sounding tools can tell us some interesting things about the aromatic compounds in coffee. For one, there's an aromatic similarity between ladybugs and a particular coffee defect (more about that later). What's more, these tools have been used to define cup quality and to train cuppers, producers and coffee-industry professionals to identify and articulate aromatic components of the coffee cup.

At the Iowa State University Olfactometry Laboratory at the Department of Agricultural & Biosystems Engineering, SPME and mdGC-MS-O processes were applied to samples of selected coffees. This article describes the processes and discusses ways in which the techniques and their output can be adapted to the unique needs of the coffee industry.

> THE TECHNIQUES

Before we delve into the details, let's examine these specific air-quality tools. Gas chromatography (GC) is a technique used to analyze the components of a gas compound. With mass-spectrometry (MS), compounds can be directly identified at the molecular level based on unique characteristics (the mass-to-charge ratio of particles). Basically, mdGC-MS-O allows the chemicals present in a complex sample to be distinguished and individually analyzed.

Moving on, solid phase microextraction (SPME) is a technique for transforming solid samples into gas compounds for analysis with mdGC-MS-O without destroying or altering the concentrations of volatile organic compounds in the sample. SPME is especially useful in field settings, because the sample preparation does not require specialized training, and the resulting extractions can be stored and transported stably for up to several days, until chromatography and mass spectrometry equipment is available.

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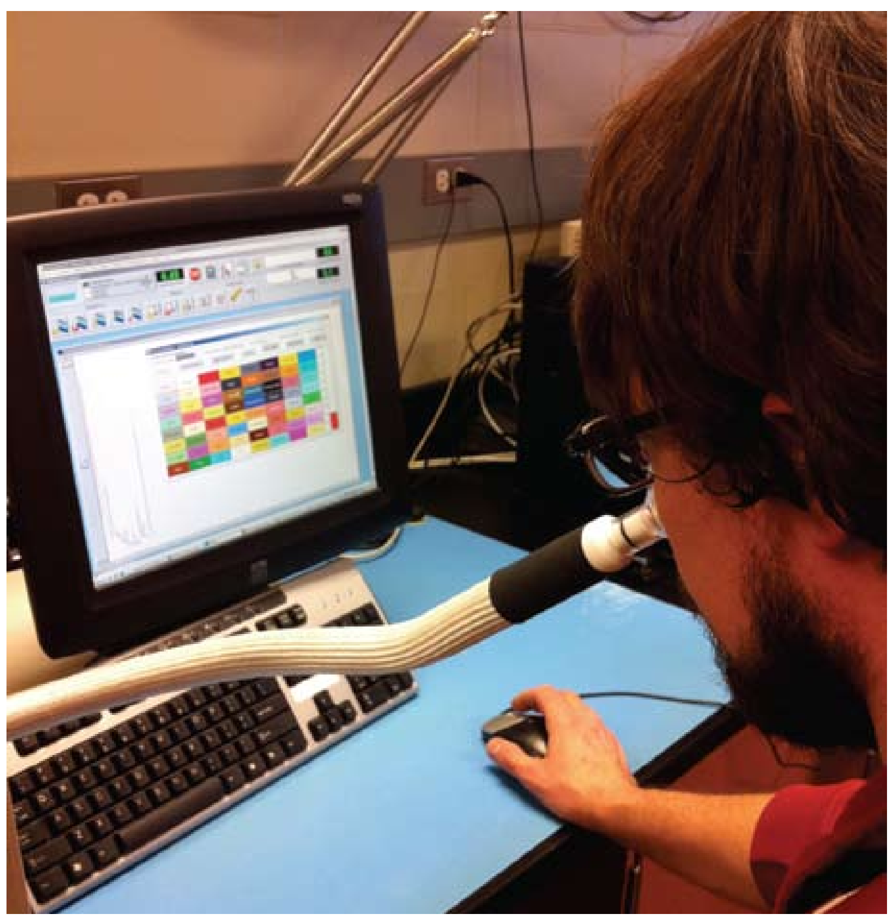
The sampling of the volatile compounds does not destroy or affect coffee beans or brewed coffee; additionally, SPME is fast and can be done without the use of solvents. When combined with chemical analyses on mdGC-MS-O, the detection limits can reach less than 1 part per trillion levels for certain aromatic compounds. SPME can be used for collection of volatiles from green beans, roasted coffee, ground coffee, and brewed coffee in the lab or in the field.

Lastly, olfactometry is a specialized application of GC-MS for identifying the molecular components of perceived odors identified by a human nose simultaneous to analysis. This makes it an ideal tool for application to coffee, chocolate, wine and beer, which display unique aromatic compounds. The technology has been around for decades. It's used in the wine industry to pinpoint when grapes should be harvested. And it's used to identify the aromatic compounds that make livestock farms stink, in order to isolate the compounds and figure out how to lessen their intensity.

SPME and mdGC-MS-O have been applied to defining coffee cup quality, in addition to demonstrating an ability to provide accurate olfactory sensory training for coffee cuppers, producers, and industry professionals. The techniques have also been used to identify the presence of defects in coffee beans.

THE BACK STORY

I learned about these air-quality innovations in October 2010 at the Global Coffee Quality Research Initiative's Congress in College Station, Texas. The Congress brought together leaders in coffee, agronomy and scientific institutions to discuss the need for scientific research on coffee quality, and to demonstrate the potential benefits of research and development. At the conference, I met Jacek Koziel, associate professor of air-quality engineering and livestock odor, who is conducting research in aromatics at Iowa State University. He shared examples of research currently being done with SPME and mdGC-



The author sniffing individual aromatic compounds in coffee.

FIGURE 1. AromaTrax computer software provides a colorful panel with a list of descriptors allowing users to record personal impressions of the aroma

MS-O, including the Rwandan potato defect, which can be identified by a compound recently discovered by Koziel. The coffee, when affected by the defect, shares an aromatic compound that had already been identified in ladybugs.

Koziel invited me and members of my team to test coffee at his lab using a simultaneous sensory and chemical analysis of coffee aroma. This approach would allow me to identify individual aromatic compound descriptors and to analyze the flavor profile of the coffees. A few weeks later, Koziel and Research Assistant Professor Lingshuang Cai met the team at the Department of Agricultural & Biosystems Engineering at Iowa State University in Ames, Iowa. Koziel was interested in learning about the industry perspective on the work being done with coffee at his lab.

We brought coffee samples for aromatic compound identification. The focus of the visit was to learn more about aromatics research, plus how the results of the coffee analysis and new research in the field might be able to improve roasting techniques. In addition, the team felt that training in olfactometry would help us to become more discerning and articulate in identifying and communicating unique flavors in our coffees.

Given that Koziel had helped discover the aromatic compound responsible for potato defect in Rwandan coffee, a few Rwandan samples were chosen for testing.

THE SAMPLING EXPERIENCE

We prepared the samples by weighing 3 grams of finely ground coffee and placing it into closed 22-milliliter vials with headspace for the aromatic properties. To start the process, a robot-like machine shakes the vial to help release the aromatic compounds, and the equipment isolates each of the compounds for the individual who will be performing the test. There could be 500 or more aromatic compounds in a sample, yet the human nose can recognize only a fraction of this number.

Next, the human aspect comes into play. The "sniff port" protrudes from the analyzer like a skinny elephant's trunk with a glass cup for the panelist's nose. One by one, the analyzer gently puffs aromatic compounds toward the sniff port. It's up to the panelist to measure the "odor activity value," or strength of a certain smell, as well as identify the type of smell (caramel or floral, for example).

In this case, the mdGC-MS-O computer program provides a colorful touch-screen panel with a list of descriptors that resembles the traditional 36 coffee-aroma panel of scents (see Figure 1 above). This allows the user to select and record personal impressions

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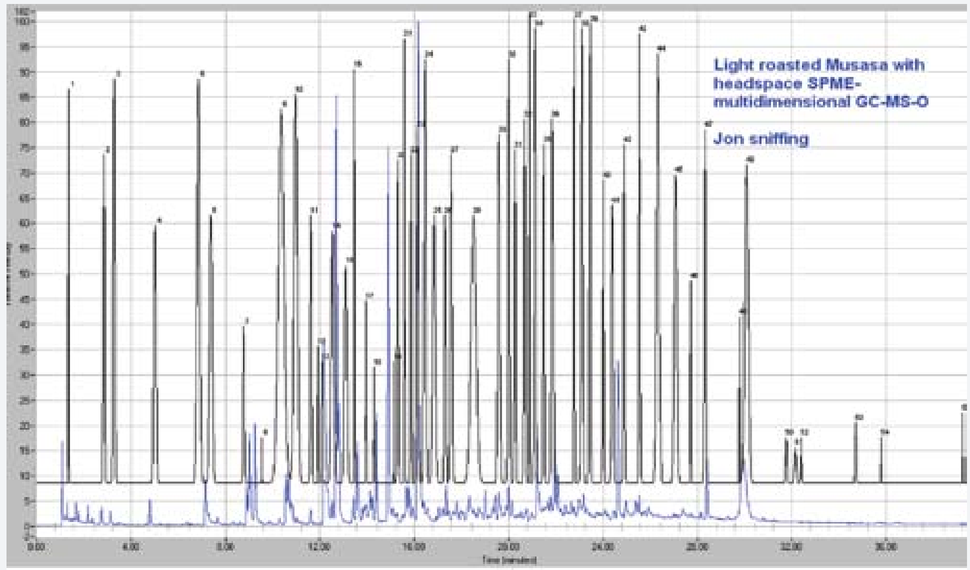
of aroma, intensity and whether the aroma is a pleasant or unpleasant sensory experience. This olfactory record creates what is known as an aromagram, which parallels with what's called a total ion chromatogram, or TIC. Much like a fingerprint, the TIC provides a unique and objective record of the aromatic compounds found in the sample. Overlaying the aromagram and chromatogram provides useful information on the linkages between certain volatiles, their concentrations with the resulting aroma character, intensity and pleasantness. (See Figures 2 and 3 this page.)

Sniffing aromas at the sniff port was like traveling in time and mapping the world of smells. The panelists experienced the same coffee aromas they work with on a daily basis, as well as new ones that were sometimes experienced back in childhood. As we discovered, responses to aromas making up coffee can be experienced and recorded by several panelists in a consistent and reproducible way.

After each coffee sample was run, Koziel and Cai provided an aromagram and gave tutorials on understanding results. After participating in a few sample tests, the panelists were better able to identify and record sensory experiences with more clarity. If an experienced cupper is introduced to this system of olfactory analysis, very little additional training may be needed to properly identify and recognize specific aromatic compounds commonly present in coffee.

FIGURE 2: Simultaneous chemical and sensory analysis of Musasa coffee by panelist 1 (blue line: chromatogram; black line: aromagram)



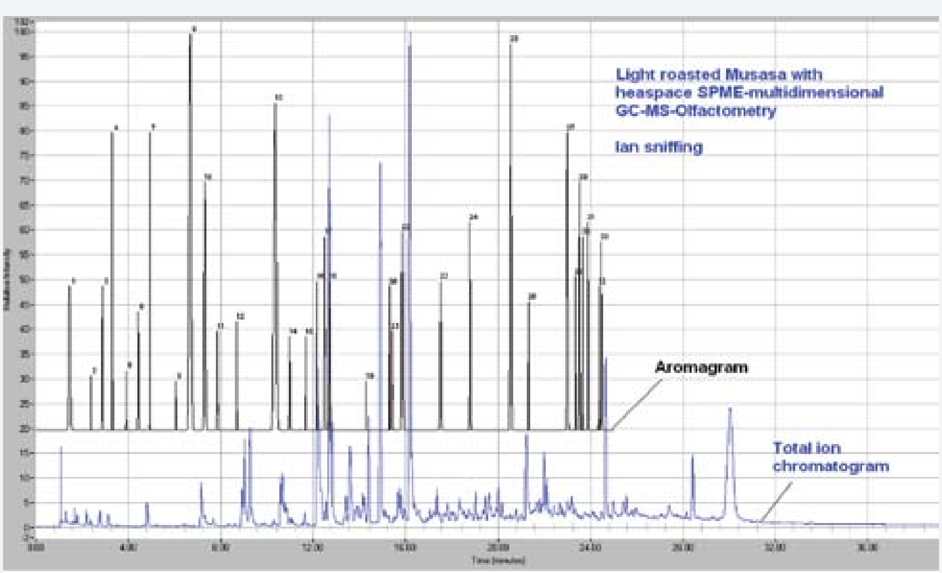
Aroma Data Acquisition: Coffee Descriptors

Simultaneous chemical and sensory analysis allows the user to sniff compounds in real time as they come out of the analyzer. The computer program (AromaTrax) provides a colorful panel with a list of descriptors allowing users to record personal impressions of the aroma. Depending on the individual panelist's viewpoint of each smell, the panelist decides whether the scent is a positive, neutral or negative experience (otherwise known as "hedonic tone"). The program also measures what's called the "event of aroma duration," or the amount of time that the aromatic compound was released into the sniff port.

The software offers the traditional 36 Le Nez Du Café aromas, along with additional senses including sulfury, burnt food, barnyard, urinous and fatty acid. The "fatty acid" and "sulfury" descriptors were useful throughout all samples. During sampling, the panelists observed the lack of ability to express more detailed sensory experiences. For example, during sampling, panelist 1 and panelist 2 both independently identified aromatics of cannabis, but were left to choose descriptors such as "animal" and "floral."

Panelists could write down the time and the sensory experience

FIGURE 3: The identical sample was later analyzed independently by panelist 2.



to be added later to the list of aroma descriptors. Additional aroma descriptors can be added, edited and rearranged, as the software allows for flexibility of working with 64 descriptors, depending on the objective and the kind of coffee being analyzed. The panelists found the option to include the ability to express "intensity" of aroma appealing and helpful.

The results from the light-roasted Rwanda Musasa, which was run for two different panelists, were of interest due to the accuracy of similar aromatic observation and expression of intensity. The panelists were not in the same room, nor had they seen each other's results before sampling began. (See Table 1 at right for a comparison of a specific aroma event experienced by two panelists.)

Here, a couple of interesting observations can be made. The similarity of sensory analysis record between two panelists who are relatively new to mdGC-MS-O is remarkable. They both sensed the same compound and, at the same time, used the same set of descriptors and agreed on the hedonic tone and intensity.

Koziel was able to explain aroma events and identify aromatic compounds responsible for some of the occurrences, using a searchable library of nearly 300,000 compounds.

Another example was the finding of an aroma similar to that of popcorn butter. This aroma is commonly associated with a potent aromatic compound—diacetyl. Table 2 summarizes the responses of two panelists to the same aroma event.

General stages of common coffee aromas in order of aromatic compound appearance during testing are summarized in Table 3.

SUGGESTIONS FOR IMPROVING TESTING

After testing, the panelists discussed the following suggestions to improve the process:

BLANK TEXT FIELD

A blank field for the observer's characteristic expression of an event would allow more detailed and timely descriptions of aromatic compounds. This was the case of the "cannabis" aroma, which the panelists were not able to immediately record during analysis. A blank field available to type a descriptor within a matter of seconds would be helpful. It would prevent a longer-than-needed search for a descriptor, causing the "duration of aroma sensation" (see Table 2) to appear longer than the actual sensory event. By the time the panelists were comfortable with a few descriptors for a particular aromatic event, the next event had already begun. Provided descriptors are vague, but it will be easier to elaborate and expand descriptors once a wider catalog of standardized aromatic compounds in coffee has been established.

IMPORTANCE OF TRAINING

Response time to an aroma event and understanding the aroma descriptors should be discussed before conducting a sample run. For example, the panelist may experience and express the olfactory sensation of "blue cheese" and not be familiar with "fatty acid" as

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TABLE 1. Comparison of the sensory analyses of "cannabis" aroma event by two panelists.

	Panelist 1	Panelist 2
Aroma event number	6	10
Time of aroma sensation during analysis	7.23 min	7.24 min
Aroma descriptor	"animal," "floral"	"animal," "floral," "malt"
Hedonic tone (pleasantness/ unpleasantness of the scale of +4 to -4)	Neutral (0)	Pleasant (+1)/ Neutral(0)
Duration of aroma sensation	0.32 min	0.15 min
Intensity of aroma on the scale from 0 to 100%	53%	50%

TABLE 2. Comparison of the sensory analyses of "popcorn butter" aroma event by two panelists.

	Panelist 1	Panelist 2
Aroma event number	4	7
Time of aroma sensation during analysis	4.88 min	4.90 min
Aroma descriptor	"butter," "maple syrup"	"butter"
Hedonic tone (pleasantness/ unpleasantness of the scale of +4 to -4)	Pleasant (+2)	Pleasant (+3)
Duration of aroma sensation	0.26 min	0.04 min
Intensity of aroma on the scale from 0 to 100%	51%	60%

TABLE 3. Summary of coffee aromas and their hedonic tones for Musasa coffee.

Stage number	Aroma characters	Hedonic tone
1	"roasted coffee," "floral," "coffee blossom," "honeyed," "butter," "tea rose"	Mostly pleasant
2	"roasted nuts," "caramel," "maple syrup," "animal," "straw," "malt," "dry vegetal," "fatty acids"	Both pleasant and unpleasant
3	"fatty acids," "cooked beef," "toasty," "pipe tobacco"	Both pleasant and unpleasant
4	"burnt foods," "toast," "chemical," "medicinal," "sulfur," "smoky," "rubber"	Mostly unpleasant

being the technical description for this aromatic compound. If the panelist was provided with an option to describe his or her sensation without restraint, such as a blank text field, this free characteristic expression of an aromatic experience may likely result in describing an aromatic compound more accurately.

Length of Sample Run

The observer must sniff a sample of coffee for a consecutive 30- to 40-minute stretch, and be prepared to properly report each aromatic event in real time as it comes out of the analyzer. Proper training on how to sniff and remain in optimal physical and mental attention was helpful. Koziel and Cai guided the panelists with detailed instructions on how to breathe and record events in a timely and proper manner. Technique for proper breathing was explained by breathing through the nasal passageway at a relaxed pace, and exhaling through the mouth. If sniffing occurs with forceful physical action, smells tend to dissipate, and after an extended period of time the observer may begin to experience physical discomforts such as dizziness and fatigue. With guidance from Koziel and Cai, it took one complete sample for panelist 1 to recognize mistakes made in the first recording, and a second sample run to understand the proper recording response procedure. Still, the pace of learning this new way of assessing coffee aroma was good, most likely due to years of experience with working with coffee and being attuned to aromas. It typically takes much longer for an average person to learn how to use this technique effectively.

Overall Olfactory Experience

An incorporation of the whole aromatic experience before or after samples that have been deconstructed into separate aromatic compounds could help. This would leave panelists with an overall cohesive aromatic impression, allowing the person to perceive what coffee smells like with all aromatic compounds present at the same time with its naturally occurring concentration levels. This could be done traditionally at cuppings but would be more accurate as a final aromatic experience to the sample run. Such a procedure would define "coffee quality" with accuracy to a given sample. Smelling aromatic parts of the whole is essential, but without recording the sensation of the whole, parts seem to be less useful. Incorporation of this overall olfactory sensation would help in controlling variables. Traditional coffee cupping has many issues to confront, such as grinding, atmospheric distractions, quality of water and time of extraction. For accurate aromatic analysis, cupping in a laboratory setting would be beneficial. Prior cupping notes of the coffee being sampled would also be of added interest in selecting samples for testing.

The Smell of Coffee

For the most part, the panelists discovered that most coffee smells terrible when you break it down into separate aromatic compounds. It's only the unique combination of these attributes that make up what most find as the attractive aroma of coffee. Using the CG-MS-O system was a "sensory-opening" opportunity, demonstrating layers of aromatics within coffee we otherwise would have never noticed or understood.

> RESEARCH, GRADING AND TRAINING

DEFINING QUALITY

Without at least a preliminary standardization of what defines quality coffee, no research can be done on the factors that contribute to a quality cup. With no scientific basis for what quality coffee is, an industry has nothing to measure quality against. Simultaneous chemical and sensory analysis allows panelists to identify specific compounds that cause certain aromas and defects. The research in aromatics at ISU can significantly launch this adventure through participation and controlled experimentation with coffee industry experts, cuppers, and sensory evaluation. Combining conventional coffee quality sensory descriptors with chemical analyses of volatile and semi-volatile compounds can provide a useful tool to separate, isolate, identify, quantify and rank specific compounds responsible for desirable quality aromas and defects. This is completed with the state-of-the-art chemical analysis that is less subjective to variations associated with sensory analyses.

One approach to begin defining coffee cup quality would be to recognize which aromatic compounds are present along with the odor activity value of each significant aromatic compound in coffees typically receiving standard Specialty Coffee Association of America (SCAA) cupping scores of 90 and above. In addition, discovering the combinations of specific aromatic compounds that together may make up specific aromas found to be pleasing to each origin of coffee would also be a task of some interest.

APPELLATION

The selection of a specific appellation for research appears to be a logical first step in defining coffee cup quality. For example, the USAID/SPREAD project in Rwanda has been working with Paul Songer, of Songer and Associates, Inc., for four years to develop appellations for Rwandan coffees. Songer informed the GCQRI and Koziel on SPREAD's latest appellation initiative using multiple samples from the North Huye region of Rwanda, taken from six farms within each of four washing station regions at different times during the harvest. Out of those, the Rwandan cuppers led by Songer selected samples that reasonably conformed to the flavor profiles developed for that region. Preliminary results from those sensory analyses confirmed the uniqueness and repeatability of the North Huye taste profile. The SPREAD team is now awaiting further analyses at Texas A&M University to determine the agronomic and geographic variables responsible for key attributes within the profile so that they can define the boundary around the North Huye "terroir" and then move on to the branding, marketing and certification stages of that appellation. Several interested coffee companies have already expressed their desire to purchase this appellation.

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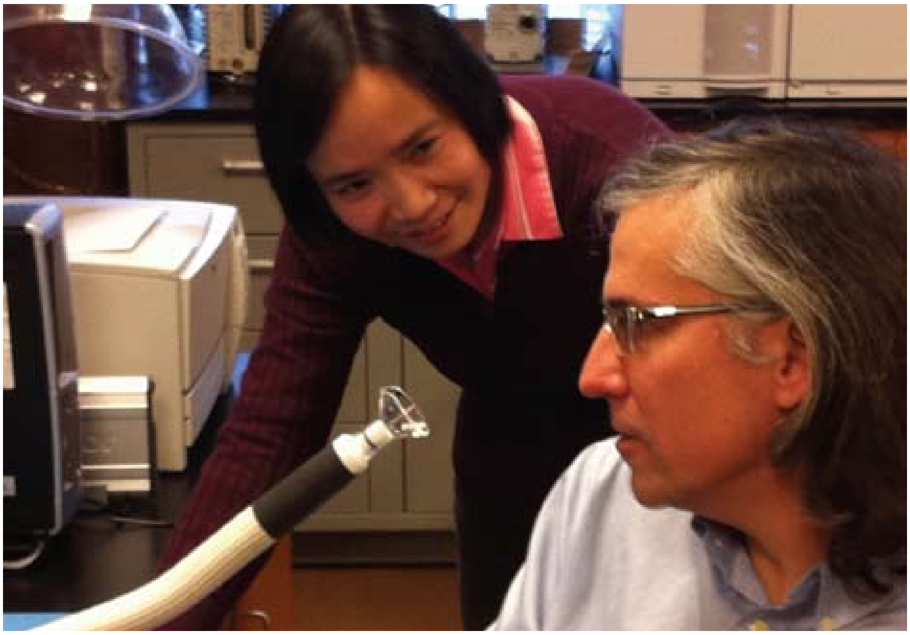
Sensory Testing

Current testing of olfactory senses used by the coffee industry seem antiquated with available technology such as the SPME and mdGC-MS-O. With this new technology, one can test an individual's ability to sense specific aromatic compounds at different concentration levels (much like the organic acids sensory exam for U.S. Barista Championship Judging, Cup of Excellence calibration session, and CQI Q-Grader exam).



Lingshuang Cai (left) and Jacek Koziel in the laboratory at Iowa State University.

As Koziel explained during the experiments, "aroma character for a compound changes with concentration." The conversation involved the concept of the odor/aroma activity value (OAV), which is a measure of importance or impact of a specific compound to the odor of a sample. OAV plays an important role in understanding the ability of humans to smell and identify aromatic compounds in coffee. If the OAV of a certain aromatic compound is too low, humans may not be able to smell a certain odor/aroma. If the concentration level is higher, one may perceive the aroma, but higher concentrations will also change the perception of the aroma.

According to Koziel, one standard (in a vial) comprised of all 36 aromatics used in the Le Nez du Café along with a selection of other common aromas found in coffee may be created to provide olfactory training for individuals within the coffee industry. In addition, the OAV of these aromatic compounds could be replicated to give proper representation in the samples.

For training purposes, the aromatics tools are capable of allowing two participants to simultaneously interact with sniff aroma compounds of the same coffee aroma sample, allowing the experienced observer to guide the student toward identifying aromas with proper descriptors. Standardization of descriptors for specific aromatic compounds may be achievable through interactive learning.

WRITING THE LANGUAGE OF COFFEE AROMATICS

Improvement of the aromatic alphabet is needed specifically for coffee-related aromatic compounds. There are traditionally 36 coffee aromas, but the alphabet could easily be expanded to be much more comprehensive, along with building a recognized vocabulary of descriptors. Ted R. Lingle's "The Cupper's Handbook" is an example of a widened vocabulary of aromatics and flavor, providing a solid beginning to standardizing an aromatic language designed specifically for coffee. Le Nez du Café falls short of some common descriptors found in most sampling. For example, "sulfur" was present in every sample tested.

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Detection of the potato defect in green coffee beans.

This seemed to be an essential addition to the list of descriptors, yet it is not included in Le Nez du Café.

The coffee industry's foundation in quality research and development is lagging behind similar beverage industries like wine, beer and spirits, specifically in the standardization and application of aromatic and flavor descriptors. The flavor wheels used within the wine and beer industries have more specific descriptors. Although many of these are often found in coffee, they are not commonly used within the coffee industry as standard descriptors.

Jacek Koziel (seated) discussing coffee aromatics with panelists in the laboratory.

QUALITY FEEDBACK

Research involving aromatic compounds has uncovered specific information responsible for the potato defect, and similar research that may be conducted on coffee will be able to inform producers which day to harvest, as well as provide information about fermentation times, storage management and proper parameters for roasting to achieve optimal flavor and aromatic attributes.

Chemical analysis represented by chromatograms are accurate, and with proper research and participation, grading coffee using similar technology would complement current Q-grading olfactory procedures for analysis. The current certification system contracts individuals who are certified Q-grader cuppers to analyze green coffee and give a score. With additional technology such as used at Iowa State University, coffee producers could receive accurate aroma fingerprints of their coffee. With additional research, producers may even be able to pinpoint certain aromatic compounds responsible for common defects in their producing area, understand how those defects affect cup quality, and learn how those defects occurred—whether it be in processing, harvesting, genetics or storage.

Jon Ferguson labeling coffee samples.

CONCLUSION

The experience visiting Koziel and Cai allowed a glimpse into the work involved in embarking on scientific research and development in coffee quality affairs. Koziel's field of study is an essential asset to research and technological development in coffee, and this lab equipment, with proper instruction and guidance, could be helpful in training those in the coffee industry to smell more accurately. In addition, the equipment could serve as an instrument to accurately evaluate one's ability to smell, much like a hearing test or eye exam.

Yet finding answers to all of these sensory issues will take considerable research and development by coffee industry professionals, and will likely not find sufficient funding through traditional government or international development organizations alone. In October 2010, a group of professionals in coffee, agronomy and scientific institutions met in College Station, Texas, to help establish the Global Coffee Quality Research Initiative (GCQRI) through forming a congress. The primary agenda was to discuss the necessity for scientific research on quality coffee. Expanding on air-quality study in the coffee industry is a prime example of research that is needed to move the industry forward.

With more research and development, less subjective descriptors and assumptions on quality will be available for debate, saving precious time to concentrate on matters of greater importance, such as whether a lightly roasted Kenyan toddy extract complements a Belgian-stye IPA. So much research, so little time.

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