THREE VARIABLES IN ONE CUP

In research funded by SCAE, Line Knutsson from the University of Copenhagen, Denmark and CoffeeMind’s Morten Münchow investigated how roast degree, extraction time and temperature affect coffee’s chemical composition.

Synopsis: Antony Watson

The chemistry behind the creation of chemical compounds that gives coffee its complex spectra of aroma and flavour is a combination of many intricately-related factors. Grind size, extraction time and brewing temperature all have a role to play in our enjoyment of a ubiquitous beverage that, worldwide, is consumed at a rate of more than 500 billion cups a year. But although the composition of coffee varies greatly from country to country, and region to region, there is one particular process that has a profound effect on its sensory qualities.

A study by Line Knutsson from University of Copenhagen, Denmark, in cooperation with Morten Münchow from CoffeeMind, into the effects of roasting degree, extraction time and temperature on coffee’s composition has revealed the extent to which the roasting process plays a vital role in the formation of a coffee’s complex chemical composition.

Commonly known as the Maillard reaction – the chemical process by which reactions occur between the amino acids (proteins) and small sugars at elevated temperatures, the study found that brewing at different temperatures (70°C, 85°C and 95°C) and extraction time (one, three, five, seven and 15 minutes) doesn’t necessarily precipitate further chemical change, rather, it is about the degree of concentration by which compounds are extracted from the freshly roasted coffee beans.

Using a washed geisha varietal grown on Las Margaritas farm, Colombia, that offers a lively acidity, creamy body, and notes of orange, mandarin, chocolate and caramel, Knutsson roasted three 1kg batches of differing roast degrees – from light, medium to dark. The three sample roasts followed the same profile with only time and final temperature varying. All samples were ground using a mill and a 1.5mm filter resulting in relatively fine particles that correspond to a medium grind size between espresso and filter coffee.

In total, 60 samples were analysed using highly sensitive techniques including Nuclear Magnetic Resonance (NMR) and Gas Chromatography-Mass Spectrometry (GC-MS) to identify the known components present in coffee. In sensory terms, NMR analyses the liquid part of the coffee, representing our sense of taste while GC-MS represents the olfactory system – or sense of smell.

Knutsson identified a whole host of chemical compounds including caffeine, chlorogenic acid, formic acid, acrylamide, trigonelline, sucrose, quinic, and acetic acid amongst others in coffee’s soluble liquid state. Similarly, a large number of volatile aromatic compounds such as pyrazines, furans and pyrroles created from the Maillard reaction were also present in the samples analysed.

The study also found a marginal difference in the coffee’s composition between 70°C, 85°C and 95°C. Similarly, different extraction times from one to 15 minutes showed that there was an impact on the concentration of aromatic substances in the samples but, overall, only a few compounds were influenced by longer extraction times.

The research shows how the extent of roast degree can have a marked difference on the chemical composition of coffee, particularly the concentration of fatty lipids and carbohydrates. Under spectromic analysis, the study found that all coffee samples consisted of acrylamide,
asparagine, acetic acid, chlorogenic acid, caffeine, myo-inositol, N-methylpyridine, sucrose, trigonelline, quinic acid and 5-HMF. In addition to these compounds, the samples contained various acids such as citric, malic and lactic acid. There were also peaks in concentration of various carbohydrates such as mannose, galactose and arabinose compounds, as well as phenol, vanillin and other coffee lipids; all products of methyl and methylene molecules from the fatty acid chains formed during the Maillard reaction.

**FLAVOUR ANALYSIS**

Nuclear Magnetic Resonance (NMR) is a spectroscopic analytic method to find the chemical structure, spatial form and electronic structure of specific molecules in its liquid or solid state. Using this form of analysis, several of the compounds that play a major role in coffee’s flavour were identified. For example, chlorogenic acid (CGA) is a polyphenol antioxidant that occurs mostly in green beans and gives a sharp, undesirable vegetal flavour. The analysis showed that concentrations of CGA are smoothed out during the roasting process, becoming less concentrated in darker roasts. As chlorogenic acid is degraded during the Maillard reaction, it converts into quinic and nicotinic acid among others which are predominant in roasted coffee. The study also confirmed that different roasting degrees have a profound effect on the coffee’s composition with the exception of caffeine and trigonelline – both relatively stable compounds that can contribute to the bitter taste in coffee.

**AROMA ANALYSIS**

Samples from light, medium and dark roasted coffee were extracted for one, three, five and 15 minutes respectively for aroma analysis. Knutsson used a highly sensitive technique of Gas Chromatography-Mass Spectrometry.
Spectrometry (GC-MS) to identify and quantify the volatile and semi-volatile organic components. Overall, 73 different substances were identified. These substances were aldehydes, alcohols, esters, furans, pyrroles and pyrazines amongst others. In particular, it is the presence of pyrazines that play an important role in the aromatic qualities of coffee.

Knutsson found that there are observable differences in the concentration of substances according to each variable change in roast degree, extraction time and brew temperature. For most substances, higher concentrations of pyridines, furans and pyrazines in darker roasted than lighter roasted beans were identified. In shorter extraction times, greater concentrations of 2-furfuryl formate were present while longer extraction times yielded higher concentrations of 3-methylbenzaldehyde, 4-methyl-1-pentanol, benzaldehyde, isoprenol and N-hexanal. In sensory terms, formate and furfuryl acetate gives a fruity aroma when perceived by the olfactory system while benzaldehyde suggests an almond-like aroma that is more consistent with darker roasted coffee.

AROMATIC ANALYSIS
Both spectroscopic methods reveal a clear correlation between roasting degree and the concentration of chemical and volatile aromatic compounds in coffee. However, there were no changes observed in the majority of compounds identified when the extraction time was varied with the exception of eight specific compounds.

These were higher levels of 2-furfuryl formate, 3,4-dihydropyran and furfuryl acetate in shorter brew times while greater concentrations of N-hexanal, isoprenol, benzaldehyde and 3-methyl-benzaldehyde were identified when the extraction time was extended.

CONCLUSION
The research highlights the role of the Maillard reaction as the prime factor in the formation of hundreds of chemical and volatile compounds present in coffee. Knutsson concludes that the research into both the aroma and liquid phase of coffee using GC-MS and NRM techniques shows that roasting degree is vital to accelerating the formation of the chemical ingredients that characterises the complexity of an individual coffee’s character.

By comparing the different concentrations of substances influenced by three variables, the study reveals that roast degree has the most significant impact in the chemical composition of the overall cup profile. Although extraction time and temperature were assessed, the significance of these variables was too small and vague to be able to make a definitive conclusion. However, there is a tendency that a longer extraction time and higher temperatures do yield a higher concentration of soluble chemical compounds present in coffee. As far as volatile aromatic compounds are concerned, only a small number of compounds were affected by extraction time.

Although it cannot be concluded if shorter brewing times and lower temperatures can be modulated for optimum commercial use – thereby achieving energy savings and a reduction in environmental impact – choosing the correct roasting degree to enhance the desired concentration of amino acids and chemical compounds during the Maillard reaction is a complex process that we are only truly beginning to fully understand.

MEET MAILLARD
More than a century ago, the French physician and chemist Louis Camille Maillard studied the complex reactions that take place between amino acids and carbohydrate sugar compounds. In 1912, he published a paper that first described this important phenomenon that takes place in the cooking of foodstuffs – and indeed our own bodies. In doing so, he prepared the way for our understanding of the browning process that gives culinary products – including coffee – its desirable colour, flavour and complexity of aroma.