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Review

Coffee: Lighting Its Complex Ground Truth and Percolating Its Molecular Brew

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Abstract: Coffee is one of the most widely traded commodities worldwide and its popularity is only increasing. The International Coffee Organisation (ICO) reported a 6% increase in global production in 2020 to 10.5 million tonnes. Coffee production is quite involved (from sowing to harvesting, processing, packaging, and storage); consequently, the industry faces major challenges in terms of the assessment of its quality, flavour, and the components which contribute to coffee's characterisation, as well as the sustainability of coffee production and global trade. This has prompted multiple studies on the nature of the aroma and taste of the many varieties of coffee around the world, which has resulted in the identification of approximately 1000 volatile compounds and the development and implementation of upwards of 100 lexicons to describe the specific sensory characteristics of coffee. The complex nature of coffee has necessitated the development and incorporation of new analytical methodologies, such as multidimensional separation technologies and spectroscopy coupled with multivariant analysis, to qualify the essential characteristics of coffee's flavour. This work aims to review the research on coffee's flavour, covering the roasting process of coffee beans, the volatile and non-volatile components generated by this process, and the chemical reactions responsible for their formation, as well as coffee's sustainability, the coffee value chain, and various forms of regulation, particularly the current emphasis on 'fair trade'.

Keywords: coffee; analytical methods; chemometrics; quality; roasting; volatile and non-volatile compounds

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1. Introduction

The popularity of coffee as a beverage, combined with the importance of its associated raw materials in terms of international trade compounds, necessitates a comprehensive and robust means of assessing its characteristic attributes. Indeed, quality is a major aspect of the modern coffee industry in its endeavour to supply the consumer with a consistently high-class product at an affordable price. The rising demand for coffee, as well as current environmental effects on the crop, is giving rise to an influx of 'bulking' or adulteration, which is using cheaper alternative grains to increase the mass of the product to add value. Additionally, the surge in demand for specialty coffee is increasing the pressure on testing, which can lead to rushed processes and lower vigilance. According to the European Ministry of Foreign Affairs, the increase in the popularity of coffee has led to mandatory environmental, social, and economic requirements associated with its production and distribution [1]. Streamlining testing procedures would allow for more frequent batch testing, increasing the economic value and giving the consumer additional confidence in the product.

The literature review conducted for this article focused on the current common practices in the analysis of coffee and the roasting procedures. The online databases used for this review included Sciencedirect, Googlescholar, and the Technological University Dublin Library Services. The primary time range of interest for this review was 2015–2024, with the exception of older fundamental papers cited to give a relevant background to coffee production and analysis. The selection of publications for review considered the scope of the analysis being carried out, the volatiles produced by coffee, the relation of these volatile compounds to flavour notes, and the effects of the coffee treatment on the presence of these volatiles. Publications relating to the health/physiological effects of coffee were not taken into consideration for this review. Key words used in online database searches included but were not limited to; coffee: -roasting, -production, -analysis, -quality control, -monitoring, -volatiles (analysis), -bean thermal analysis, coffee gas chromatography, coffee liquid chromatography, and coffee (volatiles) spectroscopy.

2. History and Origin

Multiple legends have percolated regarding coffee and its discovery, the earliest being its divine introduction through the prophet Mohammed, while the best known is the discovery of the coffee plant by Kaldi [2,3] and his goats in the hills around a monastery on the banks of the Red Sea. The first documented mention of coffee was around 900 AD by Razes, a 10th-century Arabian physician, who noted it as "hot and dry and very good for the stomach"; however, cultivation of coffee is estimated to have begun as early as 575 AD.

The beverage is a product of the roasted seeds of the *Coffea Rubiaceae*, a tropical woody genus belonging to the *Rubiaceae* family [4,5]. Antoine de Jussieu was the first to provide a botanical description of the coffee tree in 1737 [4], initially as *Jasminum arabicanum* and later as *Coffea arabica* under the genus *Coffea*.

The dissemination of coffee plants across the world from Ethiopia resulted in the development of multiple novel cultivars through the hybridisation of selected varieties to produce plants of greater robustness, productivity, disease resistance, and superior grades. Moreover, with the discovery of new wild varieties, there are over one hundred catalogued species within the genus *Coffea* [5–8], of which the United States National Centre for Biotechnology Information (NCBI) has reported that just twenty-five have been extensively studied [7,9].

Of the various species of the *genus Coffea*, two varieties are economically and commercially important: *Coffea arabica* (arabica coffee) and *Coffea canephora* (robusta coffee) [10,11]. These differ from a botanical perspective (Table 1) and in terms of their signature attributes (Table 2).

Table 1. Botanical classification of coffee [4,9,12,13].

Kingdom	**Vegetable**
Subkingdom	*Angiospermae*
Class	*Dicotyledoneae*
Subclass	*Sympetalae* or *Metachlamydeae*
Order	*Rubiales*
Family	*Rubiaceae*
Genus	*Coffea*
Subgenus	*Eucoffea*

Within the industry, Arabica beans are more valued due to their finer flavour, which is preferred to robusta by most consumers. Currently, most commercially available coffee beverages are produced either from roasted beans of arabica, robusta, or blends of the two varieties. A third commercial species, *Coffea liberica*, is also produced commercially, although on a much smaller scale. Geographically, coffee is primarily grown between 22 and 26° N, with coffee seed germination taking 1–2 months [14]. Coffee plants take approximately 3 years to begin producing fruit [15]. Cultivated coffee trees have a lifespan of around 30 years [16]. Certain species are more prone to 'rust', which refers to a condition where the *Hemileia vastatrix* fungus attacks the leaves of the trees, causing them to turn yellow and die, which can lead to the decline and ultimate death of the tree [17]. The plant flowers for up to two weeks, followed by the development of coffee cherries. Arabica cherries take between 6 and 9 months to ripen, while Robusta requires 9 to 11 months [14]. When matured and ready to harvest, the berries turn from green to yellow (*coffea arabica nana*) or a deep red. Once the berries are ripe, there are three main methods for bean preparation, which all result in varied flavour profiles: dry, semi-dry, and wet. These methods refer to the degree to which the berry pulp is removed from the remaining coffee bean prior to the drying stage of the process [18]. Dry coffees are often associated with a sweeter full-bodied taste, while on the other side of the spectrum, the wet process produces a more acidic and bitter flavour [19].

Coffea arabica (Arabica) is preferred by consumers over *Coffea canephora* (Robusta) due to the difference in flavour, which is a consequence of the variance in constituents such as the amount of sugars and acids present in each variety (Arabica varieties contain almost twice as much sucrose as Robusta) and the lipid concentration [20]. Lipids such as triglycerides, free fatty acids, and esterified diterpenes constitute about 7–17% of the dry weight of coffee beans, depending on the variety [21]. The presence of sugars and lipids in coffee contributes to the development of a sweet and smooth flavour during the roasting process, while the acids balance out the flavour and contribute to the signature bitterness of coffee. The sensory profiles of different coffees are the product of contrasts between varieties, growth conditions (e.g., altitude, rainfall, and sunlight), processing variables (e.g., fermentation, drying, and roasting), and packaging, storage, and brewing conditions.

The huge surge in the popularity of coffee in the last several years has seen the rise of 'specialty coffee'. This is a term used to emphasise the calibre and origin of a given product. Such coffees usually command higher market prices due to the perceived superiority of the beans. In terms of standards, previously, coffee had to be palatable at a minimum. However, with the rise of speciality coffee, quality and consistency have become priorities [22–26]. The Specialty Coffee Association (SCA) has developed a scoring system called the Coffee Value Assessment (CVA) in order to rank coffee attributes. This involves the ranking of coffee using factors such as aroma, fragrance, aftertaste, acidity, and cup uniformity, among others, in order to generate a score out of a total of 100 points. Coffees that score above 80 on the CVA are considered as specialty coffees. These coffee beans are normally produced in smaller batches and have unique tasting notes. Arabica beans are most commonly used as they are known for their versatility and their flavour, which is said to be easily influenced by the harvesting and roasting process [27–30]. It is important to establish mechanisms that allow for assurance and evaluation, followed by certification of products, to maintain market and commercial competitiveness.

3. The Coffee Roasting Process

Research has been carried out to correlate coffee class with the physiochemical characteristics and the chemical composition of green or roasted beans; it is important to differentiate between the raw material (green coffee) from the final product (roasted coffee) [31–34].

Table 2. Main characteristics of commercially relevant coffee varieties [4,31,35,36].

Species	**Variety**	**Origin**	**Characteristics**		
			Growth Habit	**Rust Resistance**	**Cup Quality**
Coffea arabica	*Typica*	Yemen	Upright, vigorous	Very poor	Excellent
Coffea arabica	Java	Indonesia	Upright, vigorous	Very poor	Excellent

Table 2. *Cont.*

Species	**Variety**	**Origin**	**Characteristics**		
			Growth Habit	**Rust Resistance**	**Cup Quality**
Coffea arabica	Bourbon	Brazil	Semi-dwarf, dense foliage	Very poor	Fair
Coffea canephora	Kouilouensis or conillon	Brazil	Tall	Resistant	Lower quality
Natural hybrid of Coffea arabica and Coffea liberica	S795	India	Tall, upright, and open	Susceptible, more tolerant with careful selection	Excellent
Cross between caturra and mundo novo varieties	Catuai	Brazil	Semi-dwarf, dense foliage	Very poor	Good; good bean size
Cross between timor and caturra coffee	Catimor	Colombia	Semi-dwarf, compact	Resistant to all races once careful selection is maintained	Fair/poor
Cross between typica and bourbon coffee	Mundo novo	Brazil	Semi-dwarf	Very poor	Excellent

Chambers developed a sensory lexicon for brewed coffee using more than a hundred different coffee samples from fourteen countries around the world [35]. The complexity of coffee aroma was linked to the diverse chemical composition, comprising over one thousand volatile compounds [35,37].

Previous efforts to identify contributors of specific aroma descriptors, chemical descriptions of the variations of coffee aroma under different conditions, and attempts to artificially recreate authentic coffee flavours have all encountered significant barriers due to the limitations of analytical technology [38–41]. The use of methods such as gas chromatography (GC) requires sophisticated equipment, improved sample preparation, and novel approaches to data analysis, limiting infield/on-site/in-process analysis [42,43]. The challenges in the approaches to the analysis of coffee volatiles can be appreciated when the complicated agricultural and supply chain pathway is considered, as illustrated in Figure 1.

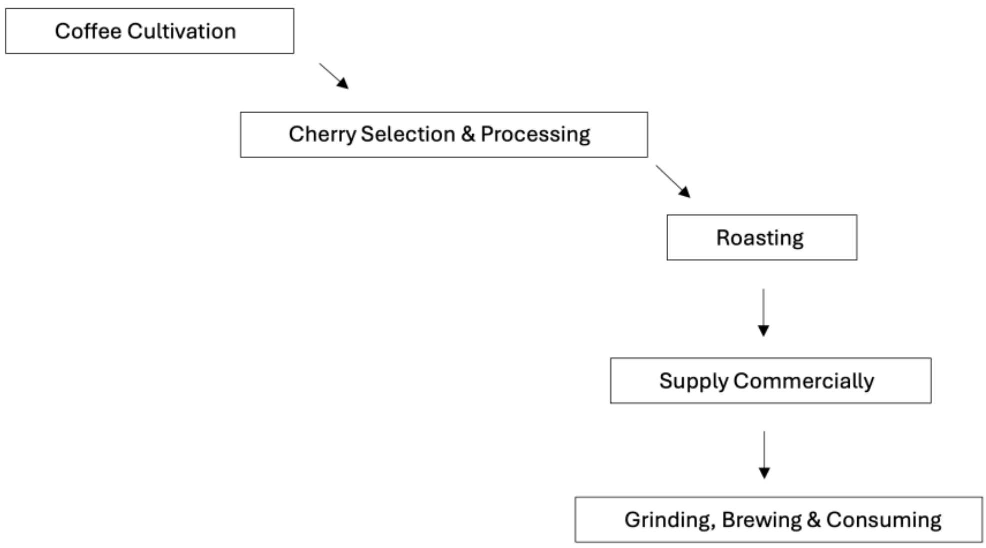

Figure 1. Key events during the coffee production process [44].

The coffee production process requires a series of intricate steps, as shown in Figure 1. Once the coffee is harvested and processed, it can then be roasted for mainstream consumption. The roasting step involves heating green coffee beans in a rotating drum, which ensures that the beans are roasted at the same rate, until the desired level of roast is reached. The beans are heated in a roaster until they reach a temperature between 188 °C to 282 °C. The rate at which they reach this temperature is known as the rate of rise (ROR) and has an impact on the overall roast [45]. Roasting times can last up to twenty minutes [46–49]. As the beans heat up, their colour slowly shifts from green to a shade of yellow before progressing to different shades of brown depending on the darkness of the roast. They emit a grassy smell as they begin roasting, and their scent slowly evolves into the deep aroma that is characteristic of coffee. The beans also 'crack' during the process [50–52]. This phenomenon is an audible cracking sound that is a result of the individual beans losing moisture due to the temperature increase.

Cracking is a signature and vital step in the roasting process. As the coffee beans roast, they can experience more than one 'cracking' stage based on the depth of roast being reached [48,49,53,54]. Light roasts of coffee normally only go through one 'cracking' step. However, green beans intended for dark roasts are heated beyond the second 'cracking' step. The darker the roast, the deeper the colour of the beans. Caramelisation of the beans also occurs past a certain temperature and the darker the roast, the more oils are released from the beans. Once the heating process is complete, the beans are then rapidly cooled, a process also known as quenching, to inhibit further roasting from residual heat [3,28,46,48,50,53,55]. The level of the roast plays a crucial role in the flavour of the coffee. Lighter roasts are generally said to be more acidic with fruity and floral tasting notes, whereas darker roasts are known to be more bitter and smoky, with caramel and chocolate tasting notes. The exact temperatures of the roasting processes are specific to individual companies and roasters, in an effort to impart unique flavours into their beans, making them stand out on the market.

The transformation of the coffee bean as it undergoes the roasting process can be attributed to a chemical process known as the Maillard reaction [56–59], which imparts rich flavours of caramel, burnt sugar, and almonds on the beans [60] (Figure 2). This occurs when amino acids and reducing sugars are exposed to heat, and it is known for browning food and deepening flavours. Common examples include the formation of crusts on baked goods, the caramelisation of sugar for confectionary production, and the roasting of coffee beans.

When the roasting process of coffee beans begins, the reducing sugars react with the amino acids, forming intermediate Amadori compounds [58]. As the reaction continues to progress and additional heat is applied, the Amadori intermediates break down and release water and carbon dioxide [59]. This, as mentioned above, is referred to as 'cracking' and causes the bean to expand [50–52,59]. The progression of the reaction causes the release of volatiles such as pyrazine-, aldehyde-, ketone-, and furan-containing compounds, which all contribute to the distinguishable taste of coffee [61]. The levels of various volatiles released depend on the type of roast, the temperatures reached, the duration of the roast, and the bean variety, as well as bean preparation prior to roasting [46]. During the reaction, melanoidins are produced, which are linked to the browning of the coffee beans [58]. Due to the heat applied, the sugars in the beans also undergo caramelisation, which contributes to the flavour profile of the finished product.

The contribution and interplay of the multiple reactions and their impact on the final coffee aroma are key to where our research would add value. Pau et al. identified three main obstacles to coffee analysis due to its matrix complexity [44], namely:

1. Coffee's complex background matrix.
2. The multiclass and isomeric nature of its volatile fraction, and
3. Its wide compound dynamic range, which encompasses important trace aroma compounds.

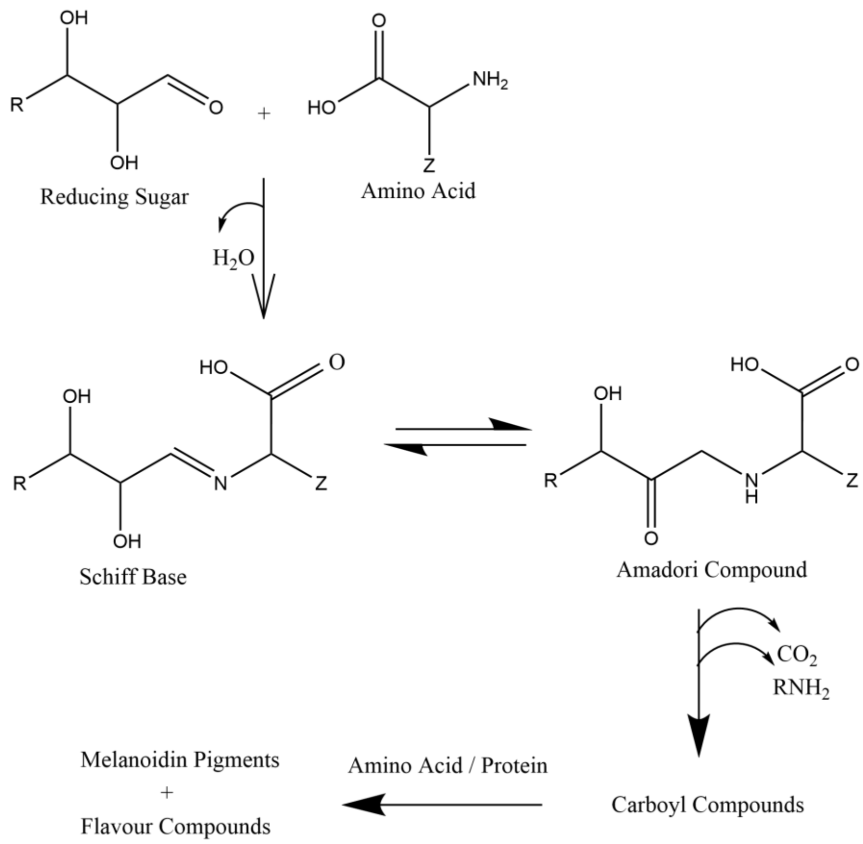

Figure 2. Simplified Maillard reaction of production formation [62].

4. Brewing Coffee

The type and standard of the roasting process play a significant role in the resulting brew. There are countless methods of brewing coffee, which are often regionally and culturally specific. They include methods such as the traditional espresso, drip coffee, stovetop 'moka pot', and French press. Newer methods such as the AeroPress® and Chemex® have now also gained popularity. Each method produces a different flavour profile. These methods also often need different grind sizes, meaning some methods are more sensitive to the less front-facing flavour notes [29,63–66].

Espressos are extracted by pushing hot water at a relatively low pressure, typically about 9 to 10 bars, through finely ground coffee beans [64]. This results in a strong, dark, concentrated coffee. It can be consumed as a short beverage without any additions but is currently more widely used as the base of drinks such as lattes and cappuccinos. The espresso and its milk-based variations originated in Italy but have gained worldwide popularity thanks to internationally recognised franchises such as Starbucks® and Costa Coffee™.

The stovetop 'moka pot' operates on a similar pressure-based principle. When heat from the stove is applied to the moka pot's lower water-filled chamber, the pressure builds and ultimately forces the water up through the coffee 'puck' in the middle chamber, with the resulting espresso-like beverage finally being collected in the uppermost portion [67].

Drip or filter coffee is made by gradually pouring hot water over ground coffee beans in a paper filter. The water then slowly drips through the grounds and into a pot or cup below [68]. This technique results in a mild flavour, usually a larger volume of coffee, and a lighter colour. Automatic drip coffee machines are largely popular in the United States, whereas Europeans have heavily embraced manual methods such as the Chemex® and V60 pour-over trends. The Chemex® is an hourglass-shaped glass carafe, where a coffee filter is applied to the top portion, ground coffee is placed into the filter, and hot water is slowly poured over the surface by hand [27].

The French press employs a plunger technique. The coffee is made by adding ground beans to the glass portion and submerging them in the corresponding volume of hot water. After several minutes, a plunger is used to press the coffee grounds down and end the brewing process, allowing the resulting brewed coffee to be poured without the grounds being also transferred to the cup. Coffee made using a French press has the potential to be more intense than other methods, as the strength can easily be increased by prolonging the time before plunging [64].

The newly popularised AeroPress® system works on a number of principles and shares some similarities to the French press, drip coffee, and traditional espresso brewing methods. First, coffee grounds and hot water are added to the AeroPress® and left to sit for a set period of time, similar to in a French press. The brewed coffee is then separated from the grounds by forcing the water through a paper filter (similar to the filters used in drip coffee methods, but much smaller in size) [64]. This passage of the water through the filter is achieved by the user manually pushing on the AeroPress® as if it were a large syringe, a stage in the process reminiscent of the pressurised brewing of the traditional espresso and 'moka pot'.

5. Economic Impact

Coffee is commercially produced in more than 50 countries and the world drinks upwards of 3 billion cups a day [69]. The annual revenue of the coffee sector is estimated to exceed USD 200 billion. The global coffee market amounted to USD 472.5 billion in 2022, with an expected growth between 2022 and 2025 of 5.28% compound annual growth rate (CAGR) and total global exports of 13.16 million bags [70]. The International Coffee Organisation (ICO) warns of market shifts due to a potential global economic downturn, increased production costs, and reduced consumption and imports due to the Russia–Ukraine conflict [71–73]. However, a survey carried out by Lanfranchi, Giannetto, and Dimitrova in 2016 showed that consumption of coffee had not suffered in recent economic downturns [74]. Brazil is the leading country in coffee production, producing over 4 million kilograms in 2020, which accounted for BRL 14.3 billion of the country's revenue in the same year [75–80], and it has been the most important coffee exporter since 1995 [81]. The United States currently leads the ranks in terms of coffee imports and domestic consumption [55], with most nations of the world having high rates of coffee consumption and a preferred brewing method [82].

6. Adulteration, Fraud, and Consumer Safety

As discussed in the previous section, coffee is widely popular and its reach is growing. As with any hyper-popular item, coffee is prone to adulteration [83]. While trained individuals can easily distinguish the physiological differences (size and colour) between raw arabica and robusta beans, the processing steps required in standard coffee production, including roasting and milling, eliminate such visual indicators. Moreover, this could result in fraudulent or accidental mislabelling, a subject of concern for food processors and regulatory authorities prompting the requirement of alternative methods for the identification of ground roast coffees [84–87]. It is vital to monitor the consistency of the product throughout the supply chain. The chemical constituents of the roasted beans determine the attributes of coffee as a beverage. Raw coffee beans contain a wide range of different chemical compounds, which react and interact amongst themselves at all stages of coffee roasting, resulting in greatly diverse final products. For instance, caffeine content, which has a significant effect on the final grade of coffee products, needs to be determined quickly and reliably by analytical techniques [88–90]. Due to the high number of samples to be analysed, the coffee industry needs new analytical techniques to provide fast and reliable data indicative of the coffee's standard [88–90].

The increasing popularity and demand for coffee raises the possibility of fraudulent or accidental mislabelling, a subject of concern to food processors and regulatory authorities [85,91,92]. Thus, it is important that the varieties of raw beans and various coffee products can be properly identified. Cheaper materials are often used in order to bulk up the final product. Commonly used adulterants include legumes, grains (barley, maize, and rye), twigs, and husks, as these are inexpensive and can, at a glance, blend in with the overall morphology of a coffee bean [84–87]. Adulteration can also involve inferior coffee beans that are cheaper and easier to grow and cultivate. This, although not inherently harmful to the consumer's health, lowers the calibre of the final product, unbeknownst to the consumer who is likely paying a premium price [65,72,79,80,85,93].

There are regulations in place in order to limit and remove adulterated or fraudulent coffee products from the supply chain. The International Coffee Council (ICC) has set out a documentational standard for the export of coffee, as outlined by Toci, Farah, Pezza, and Pezza [87]. The coffee is not permitted to have an excess of 89–150 defects per 300 g, depending on the bean variety. Brazil, the leading exporter of coffee in the world, has its own stringent laws in place, which have a 1% limit for the combined content of the above-mentioned impurities [25,94]. Chromatography-based techniques, in particular gas and liquid chromatography, along with mass spectrometry and infrared spectroscopy, are commonly used in adulterant detection [87,90,95–97]. Adulterant analysis and detection using these methods involve the identification of compounds such as glucose, xylose, mannose, and starch [87,90,95–97].

Fairtrade is another accreditation that plays a significant role in coffee cultivation. Fairtrade Ireland defines the organisation as a 'partnership between some of the most disadvantaged farmers and workers in the developing world and the people who buy their products'. The label stands for standards and ethics that include fair wages to workers, fair labour conditions, environmental sustainability, and community development for the communities in which it operates [97–99]. The organisation, along with its seal of approval, is a sign to consumers that the product is grown and cultivated to a high standard.

7. Standard Methods of Analysis

The analysis of coffee odorants spans from the volatiles released and developed during the roasting process to those extracted during brewing, encapsulating many factors in between such as roast, storage, grinding method, and brew method [38,39,44,98,100,101]. Studies of coffee odorants have found that some of the most common compounds contributing to the flavour profile of coffee are alkyl pyrazines, furanones, Strecker aldehydes, furans, and phenols [102].

7.1. Chromatography

Chromatographic methods of separation and analysis of coffee help manufacturers optimise their process to produce coffee with specific taste and aroma profiles. It is a powerful tool that can assist analysts in understanding the chemistry of coffee and improving the characteristics of coffee products. Various methods of analysing coffee using chromatographic techniques have been investigated since the early 1970s, beginning with thin layer chromatography (TLC) and progressing onto ion chromatography, high-pressure liquid chromatography (HPLC) [103], and gas chromatography (GC), with some other variations such as head space samples and mass spectrometry (MS) detectors [104]. Solid-phase microextraction–gas chromatography (SPME–GC) was used in the 1990s to characterise roasted coffee using principal component analysis (PCA) [105]. Gas chromatography olfactometry with mass spectrometry has also been used for sensory analysis to investigate the appeal of certain compounds to consumers [39]. As chromatographic methods are both well-established and reviewed (highlighting their capabilities), they are briefly explored here to establish a baseline for common techniques currently in use [39,44,98,102,104,106–108]. Moreover, the authors would encourage readers to explore the works of those we cite throughout.

Chromatography is often used in food-related quality control analysis in the production of oils, wines, and spirits. Through the use of different chromatographic techniques, manufacturers can monitor the chemical composition of coffee during the processing of the fruit and roasting of the beans. Coffee is widely known and recognised for its specific aroma, and these signature and strong odours make it a good candidate for gas/vapour analysis, with methods such as headspace GC, which samples these vapours alone [104]. The information gathered through chromatographic analysis can help in adjusting the roasting parameters to bring out and enhance specific flavour profiles based on the presence of corresponding flavonoid compounds.

A study by Czerny and Grosch, which used gas chromatographic methods, monitored some common coffee odorants such as 3-isobutyl-2-methoxypyrazine and 2-Methoxy-3,5-dimethylpyrazine through the roasting process and saw the concentration increase in roasted beans, bringing out the signature, sought after coffee aroma [100]. Analysis of the elemental composition of coffee has also been conducted using flame atomic absorption spectrometry (FAAS) and inductively coupled plasma optical emission spectrometry (ICP-OES), among other techniques, to examine the differences between green and roasted coffee beans. This found that the elemental composition varied more based on geographical location and soil type than the roasting process [109]. Once roasted, the coarseness of the grind of coffee can have a major impact on the flavour profile of the final beverage, with a comparative odour decrease in coarser ground coffee compared to a finer grind [110]. Furthermore, if the intended product is instant coffee, the beans then undergo an extraction process that essentially draws out all the 'trademark' coffee constituents in water, which is then commonly frozen or evaporated to intensify the concentration [106].

Chromatography is also widely used within the food production industry to screen for and detect adulteration, discussed in Section 6, and inferior products. Even after grinding the coffee beans, chromatography can identify the presence of adulterants such as chicory or soybean [87]. Similarly, this application can also be used to authenticate coffee bean type and origin. Geographical locations that traditionally produce coffee can impart unique flavour and aroma profiles onto the fruit and later the bean. These unique traits can be attributed to environmental conditions such as general climate and soil conditions [111]. Chromatography, specifically variations of gas chromatography, is also being used to study the impact of different processing methods and roasting profiles on the chemical composition of coffee. Typical identified volatile coffee components include, but are not limited to, acetates, acids, alcohols, aldehydes, esters, furans, ketones, lactones, monoterpenes, phenols, pyrazine, sulphides, and thiols [107].

Gas chromatography is a robust method for the analysis of coffee beans throughout their production. However, it is limited in that it requires extremely specialised equipment with trained personnel to carry out the analysis. It is also time-consuming and expensive, making it often inaccessible to smaller coffee producers. It is also limited in terms of the types of compounds it can detect [44]. Compounds such as proteins and carbohydrates, which cannot be volatilised, will not be detected, meaning it is optimally combined with other techniques, such as spectroscopy and the chemometric interpretation of data [112].

7.2. Infrared Spectroscopy

Spectroscopic techniques have several advantages over other analytical techniques used in food production, specifically coffee analysis. One of the main advantages is the speed of the analysis, as it can analyse the sample in a matter of seconds, making it a rapid technique for standard surveys in coffee production that can be implemented at any stage of the process without interfering with the chain of events. It is also non-destructive in nature, does not require sample preparation, and the sample can be small, which is particularly useful in instances where the producing body is a small operation. It is also cost-effective, as it does not need expensive chemicals and preparation techniques or staff in order to carry out the analysis [68]. It has been used for the analysis of coffee components for a variety of purposes. Barrios-Rodríguez et al. carried out FTIR analysis in conjunction with chemometrics in order to study the effects of harvesting methods on coffee [113]. Chemometrics were then employed, based on PCA discrimination, in order to identify the highest-calibre coffee as defined by the Specialty Coffee Association (SCA). Classifications were made and categorised based on the absorbance for the following wavelengths: 2925, 2850, 1740, 1650, 1602, 1550, 1300, 1252, and 1150 cm^{-1}. Chemometrics and multivariate analyses are commonly used in combination with spectroscopic techniques and can be used to calculate the contribution of a specific compound to the spectrum [114].

The chemical composition of coffee can be analysed using IR, based on the absorption of infrared radiation by different molecules within the coffee matrix at specific frequencies that are associated with chemical bonds present in those specific molecules [68]. Some of the representative compounds commonly analysed using IR include caffeine, trigonelline, and chlorogenic acid. These compounds play a large role in determining the grade and authenticity of coffee.

Caffeine is one of the words most commonly associated with coffee, as this is a vital and signature compound in coffee and is responsible for its well-known stimulating effects on the consumer. Spectroscopic techniques can be used to determine the caffeine content in coffee samples, which is useful as some beans can be discriminated based on their caffeine content. For example, this can be used to differentiate between arabica and robusta coffee beans, both of which vary in caffeine content [115]. Trigonelline and chlorogenic acid are two more compounds that are commonly found in coffee. Trigonelline is known to be responsible for the bitter taste of coffee, meaning the higher the trigonelline content in the bean, the more bitter the subsequent cup of coffee it produces. Chlorogenic acid is responsible for the antioxidant properties in coffee and can also be monitored using infrared spectroscopy [116].

A review by Munyendo, Njoroge, and Hitzmann [117] describes other spectroscopic techniques, such as mid-infrared, near-infrared, Raman, and fluorescence spectroscopy, used for the analysis of coffee, which, when combined, produce a wide variety of spectra associated with coffee in different states (i.e., green, light roast, dark roast, etc.) [117].

The use of near-infrared spectroscopy (NIR) to study the process of roasting coffee can be used to target specific characteristics/traits/attributes of interest. Different varieties of coffee beans will have varying compositions, even green beans, which results in variations in the roasting process. Roasted beans range in moisture content from 1.5% to 5% [118]. During roasting, the coffee beans change from green to yellow as their odours develop and deepen as temperatures increase up to 210 °C [108]. One such investigation into the roasting process and flavour/odour development, carried out by Esteban-Díez, González-Sáiz, and Pizarro [32], was able to correlate the NIR spectra obtained to the colour of the bean, linking the visual appearance to the chemical composition associated with the degree of roasting [32]. Another study by Wójcicki [119] analysed the coffee roasting process using near-infrared (NIR) spectroscopy and concluded that the beans that were roasted for a shorter period of time had a higher absorbance than the beans that were roasted for longer in all the wavelength ranges examined. The study also found a promising linear relation between the roasting power and the resulting spectra, showing promising potential for spectroscopy paired with chemometrics as a monitoring tool [119]. A review by Barbin et al. [120] on the application of these spectroscopic techniques to the analysis and monitoring of coffee predicted the further expansion of these techniques to aid regulatory inspection as an effective and inexpensive technique, which could lead to a decrease in errors and labour costs [120]. Additionally, this method of analysis can be adapted and used in order to monitor the effects of climate change and other variable factors of agricultural supplies of various grains, wheat, and legumes based on gathered datasets and statistical interpretations [121].

Spectroscopic methods are incredibly robust, allowing for rapid analysis of an array of samples. However, they are not identification methods. They are a tool that can be used for comparison, and when used with an established data bank in the area of interest, they can be used to place an unknown sample within a sample set, relative to the pre-existing data.

7.3. Thermal Analysis

Thermal analysis can be used in the quality control and assurance of coffee products in combination with other techniques. The thermally dependant behaviour of coffee during different stages of its production can give insight into the optimal roasting and brewing temperatures needed to yield a high-grade, consistent product each time. Thermal analysis of coffee is an important aspect of understanding its chemical composition and physical properties. Most food production involves a thermal analysis step. Two of the most commonly used techniques for thermal analysis in food production and quality assurance are differential scanning calorimetry (DSC) and thermogravimetric analysis (TGA) [122].

Differential scanning calorimetry is a thermal analysis technique used to measure the heat flow in a sample as a function of temperature. This technique is regularly used to study the thermal behaviour of coffee during the different stages of roasting. This technique measures the amount of energy necessary to increase the sample temperature. The resulting thermogram showcases any events occurring within the sample during the temperature changes, such as Maillard reactions, caramelisation, and pyrolysis [44]. Similarly, thermogravimetric analysis measures the mass change within a sample as a function of temperature or time. It is often used to examine the loss of mass that occurs during roasting, which is mainly due to the evaporation of water and other volatile compounds. The resulting curve can indicate the degree to which the beans are roasted and give an indication of the quantity of lost volatiles. TGA is also used to study the degradation of coffee during storage and the impact of different storage conditions on the state of the beans [123]. The authors suggest that the resulting curves could have potential as a tool for adulterant screening. Pereira et al. reported that thermogravimetric analysis was useful for screening ground coffee for adulterants such as barn, wheat, corn, and sticks [124]. Overall, thermal techniques can provide valuable information about the chemical and physical changes that occur during the roasting, storage, and brewing stages of coffee preparation. The ability to recognise and monitor these changes is crucial in maintaining production chain standards and customer assurance. However, it does not provide compound identification capabilities.

7.4. Gas Sensing (Electronic Nose)

Rodríguez et al. reported the use of electronic noses for the analysis of green beans [125]. They suggest that the technique may be adapted to monitor the coffee roasting process. In a similar study, Barea-Ramos and colleagues caution that the gas sensors utilised in electronic noses are prone to drift, which can result in variations in results even when used on the same sample in identical conditions, which may limit the potential ability of such sensor arrays and models to classify and identify coffee roasts [126].

Overall, researchers within the field of gas sensing using apparatus such as Agrinose electronic nose sensors attest that the techniques can facilitate more rapid testing than traditional GC-MS analysis. They promote such electronic nose sensing tools for the inspection, classification, and quality monitoring of coffee. However, it should be noted that such tools employ metal oxide semiconductor (MOS) sensors, which are subject to drift and lower limits of detection, to detect the target analyte gasses. Consequently, they are comparatively and significantly limited to gas chromatography–mass spectrometry [127]. This technique is more cost-effective than standard gas chromatography analysis and is being investigated as a screening tool to monitor certain VOCs resulting from the coffee roasting process [19,45,60]. In combination with machine modelling, the use of e-nose technology can automate such screening procedures and limit the need for staff involvement, limiting the impact of potential human interference [128]. However, the limitations associated with this method cannot be ignored, primarily the concentration of VOCs present acting as a limiting factor, which in turn may impede their usefulness in real-world applications.

8. Discussion and Conclusions

Recent developments in a wide range of disciplines associated with food production afford analysts a better understanding of the compositional and nutritional traits and properties of these natural products, allowing for a more holistic, interdisciplinary, and systematic approach to food analysis. The introduction of modern data analysis techniques jointly with multifaceted/multicomponent analytical techniques can be used to explain specific attributes and properties related to chemical and sensory characteristics not readily determined by classical targeted chemical analysis. The literature includes multiple works that illustrate the potential of chemometrics. In conjunction with several other techniques, chemometrics can establish a more user-friendly in-field, in-process method of monitoring the grade of the coffee throughout the entire production process to better assist relevant stakeholders. The involvement of a thermal technique, such as thermogravimetric analysis combined with infrared spectroscopy, could allow for the real-time monitoring of the evolution of coffee volatiles throughout the typical roasting process and temperature programme. The analysis can be further expanded through the use of a hyphenated system that passes the evolved volatiles during the roasting process carried out by the TGA through the IR and into a gas chromatography–mass spectrometry (GCMS) component, which will further separate out the compounds involved, allowing for a more detailed evolution timeframe and characterisation. Following this with in-depth spectroscopic analysis would allow for the development of a statistical approach and multivariate analysis for the categorisation and classification of the product as it travels down the supply chain. The optimisation of this approach could lead to the creation of a comprehensive database, which would be available to farmers, cultivators, roasters, distributors, and consumers.

Over the last several decades, coffee has established itself as a sought-after commodity across the world. With seemingly ever-growing popularity, the demand for production is growing, putting mounting pressure on producers. In order to keep up with demands, production, as well as quality control and regulations, need to be optimised. Based on the literature available to date, each step of the coffee roasting process is currently being examined separately. This produces detailed results yet is time-consuming and resource-demanding in terms of equipment, consumables, and staff. Given that the roasting process is vital in the production of coffee and coffee-based products, an inline screening solution would allow for rapid and non-destructive analysis, the results of which can be analysed and interpreted using chemometrics. This, in turn, can simplify on-site characterisation and potential fraud detection, as well as aid in monitoring standards using multivariate analysis.

The above-discussed analytical techniques provide insight into the complexity of a 'simple' cup of coffee. From cultivation to roasting, grinding, and brewing, the entire process is extremely involved, and flavour/odour development occurs at every step along the way.

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