International Journal of Food Science +Technology

Institute of Food Science +Technology ifst

Review

Effects of postharvest processing on aroma formation in roasted coffee – a review

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(Received 1 December 2022; Accepted in revised form 13 December 2022)

Summary Postharvest processing of coffee cherries significantly influences sensory characteristics and commercial values. Aroma is one of the critical elements in product qualification and differentiation of coffees from different origins, roasting levels and brewing methods. Except for primary coffee volatile organic compounds (VOCs) (furans and pyrazines), which are generated during postharvest processing (dry, honey, wet processing and roasting), aldehydes, ketones, phenols, sulphur compounds and others could also contribute to the complex coffee flavour. Desirable flavour requires a balance between pleasant and defective VOCs. This review comprehensively discussed the mechanisms of conventional and novel postharvest processing of coffee beans, their impact on the sensorial profile of green and roasted coffee, and the composition, generation and analysis techniques of coffee VOCs. This review shows the feasibility of GC–MS and electronic nose (E-nose) in coffee VOCs and flavour detection, meanwhile building a comprehensive linkage between postharvest processing and coffee sensory characteristics.

Keywords Aroma, coffee flavour, e-nose, GC–MS, postharvest processing, VOCs.

Introduction

Nowadays, coffee is the second-largest commodity in the global market after crude oil (Haile & Kang, 2019; Zakidou *et al.*, 2021). According to the International Coffee Organisation (ICO), 166.35 million (60 kg) bags of roasted coffee were consumed in 2020/2021, with a 1.0% increase compared to 2017/2018. It is also the second most consumed beverage after tea owing to its energising function and a broad spectrum of aroma and flavour. The demand for speciality coffee, made from certain varietals or specific processing methods, has been rising lately (Zakidou *et al.*, 2021). For instance, the Geisha varietal is favoured mainly because of its floral and sweet taste, while wet processing could generate more outstanding coffee sensory characteristics than dry processing. A total of 43% of consumers chose speciality coffee in 2022, with an increase of 20% compared to 2021, and reached the highest level to date (da Silva Portela *et al.*, 2022).

Generally, the genetic varietal of coffee plants and the geographic conditions could directly or indirectly influence the size, shape and chemical compositions (sugar, fat, protein) of raw coffee beans (Kitzberger *et al.*, 2016). The elements of geography and environment generally include geographic altitude, light exposure, projected temperature, water resource and precipitation regime, cultivation methods and pest and disease management (Ahmed *et al.*, 2021). Some influential aromatic makers found in roasted coffee, such as 2,3-butanedione, 2,3-pentanedione, 2-methylbutanal and 2,3-dimethyl pyrazine, could be significantly impacted by geographic variations (de Toledo *et al.*, 2017; Dryahina *et al.*, 2018). Increased light exposure could also reduce the phenolic metabolites and increase lipids content (Muschler, 2001; Delaroza *et al.*, 2017). Decazy *et al.* (2003) observed that more intensive light exposure might reduce coffee sensory quality due to the lack of aroma. Läderach *et al.* (2017) also reported an improved body of brewed coffee with expanded shade on the farm. Besides, crop quality and productivity can be impacted by the nutrients available in the soil. The potassium fertilisation practised on the farm is believed to be an essential controller to regulate many flavour-related components, such as sugars, chlorogenic acids and phenols (Clemente *et al.*, 2015; Vinecky *et al.*, 2017).

Although over 100 species have been identified worldwide, only two are most commercially valued, namely *Coffea arabica* and *Coffea robusta* (*Canephora*)

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doi:10.1111/ijfs.16261

(Davis *et al.*, 2006). Nowadays, 75% of the total coffee production in the global market is from *Arabica* spices due to their higher chemical complexity than *Robusta*, which is the potential to make roasted coffee more favourable (Toledo *et al.*, 2016). The relatively higher concentration of 2-methylisoborneol in *Robusta* is considered as a factor of its typical earthy note (Knysak, 2017). Another critical role of postharvest practice (fermentation and roasting) is regulating the conversion of these resources into distinguishing VOCs in the final cup (Toledo *et al.*, 2016; de Melo Pereira *et al.*, 2019). The choice of washed (wet), dry (natural) or semi-dry (honey) processing is considered one of the most quality-differentiative steps in the coffee production (Sunarharum *et al.*, 2014; de Melo Pereira *et al.*, 2019) since it decides the presence of de-pulping and mucilage, resulting in different chemical compositions, which functions as the aromatic precursors in the following steps (Gonzalez-Rios *et al.*, 2007a, 2007b). This is discussed in detail in the later section. Many factors need to be considered when selecting the optimal method for a specific roasting batch of coffee, including coffee species, targeted flavour, farm scale and expected cost (Lee *et al.*, 2013a; Toledo *et al.*, 2016).

Coffee cherry, the raw and unroasted coffee beans, usually possess undesirable peasy off-odours because of alkyl-methoxy pyrazines (such as 3-isobutyl-2-methoxypyrazine) (Flambeau *et al.*, 2017). Roasting can suppress these compounds and convert them into a pleasantly roasty aroma (Sunarharum *et al.*, 2014). Most of the volatile compounds (VOCs) related to the coffee aroma, including pyrazines, furans, aldehydes, ketones, phenolic compounds and sulphur-containing compounds, are principally produced from Maillard reaction, caramelisation, Strecker degradation and pyrolysis during roasting (Akiyama *et al.*, 2003; Franca *et al.*, 2005; Toledo *et al.*, 2016; Zakidou *et al.*, 2021). In roasted coffee, furans and pyrazines are arguably the most quantitative compounds. Sulphur-containing compounds (despite their relatively lower contents in roasted coffee) and pyrazines could be the most influential to the sensory quality (Sunarharum *et al.*, 2014). The mechanisms of producing these compounds are interactive and highly complex, contributing to various concentrations and unique sensory properties of brewed coffee. The health benefits of coffee consumption are always associated with its antioxidant capacity (the ability of retarding oxidative reactions), which is believed to be achieved mainly by phenolics, such as flavonoids and tannins (Haile *et al.*, 2020; Chindapan *et al.*, 2022). Ludwig *et al.* (2014) reported that heterocyclic VOCs (furans, pyrroles and thiophenes) showed the highest antioxidant activities among the detected VOCs in roasted coffee. Chlorogenic acid, one of the most abundant esters found in coffee, is reported as a good source of antioxidants consumed from dietary sources (Buffo & Cardelli-Freire, 2004). Nevertheless, the presence of aromatic furans is a concern over the possible negative impact on human liver function (EFSA Panel on Contaminants in the Food Chain (CONTAM) *et al.*, 2017, Haile *et al.*, 2020). Long-term observational investigation on the health effect of coffee consumption is still required. Due to the volatility of those compounds, analytic detection also requires high sensitivity, kinetics monitoring and trace detection (Chang *et al.*, 2016).

Coffee provides an intricate blend of various flavours after postharvest processing, roasting and brewing, which develop a range of sensory experiences. Specific sensory characteristics differentiate the types of coffee varietals, processes and roasts (Stroebaek, 2013). Generally, the human sense of smell can identify over 10 000 different odorants *via* retronasal and orthonasal systems, while the sense of taste can only distinguish five official tastes (sweet, sour, bitter, salty and umami) and two recently acknowledged basic tastes (starch and fat) (Petracco, 2001; Keast & Costanzo, 2015; Besnard *et al.*, 2016; Low *et al.*, 2017). Therefore, the coffee flavour plays a prominent role in the coffee sensory qualification as it is the mix of aromas, tastes and trigeminal sensations (Stevenson, 2012; Sunarharum *et al.*, 2014). The odours or aromas chiefly come from the VOCs produced during postharvest preparation and roasting, which will be particularly reviewed in the following sections. This review aimed to address the effect of coffee postharvest process and roasting conditions on the VOCs composition and the aroma formation in roasted coffee. The application of traditional (GC-MS) and novel sensor technologies (Electronic nose) to assess VOC is discussed. Those two methods have been widely used and validated for chemical and sensory analysis in the food and beverage industry. Besides, other methods such as Nuclear Magnetic Resonance (NMR), Proton-transfer Reaction Mass Spectrometry (PTR-MS), and Gas chromatography-olfactory (GC-O) have also been used in the industry.

Postharvesting processing

Postharvest processing with the botanical structure changes in coffee seeds is illustrated in Fig. 1. The coffee cherry pulp (mesocarp) in the middle is rich in nutrients such as carbohydrates (pectin, glucose and fructose), fat, protein and other substances, which could be the resource of aromatic compounds produced in the following processing (Janissen & Huynh, 2018; de Melo Pereira *et al.*, 2019). The endocarp is a polysaccharide layer mainly composed of cellulose, hemicellulose, lignin and ashes (Esquivel & Jimenez, 2012). Noticeably,

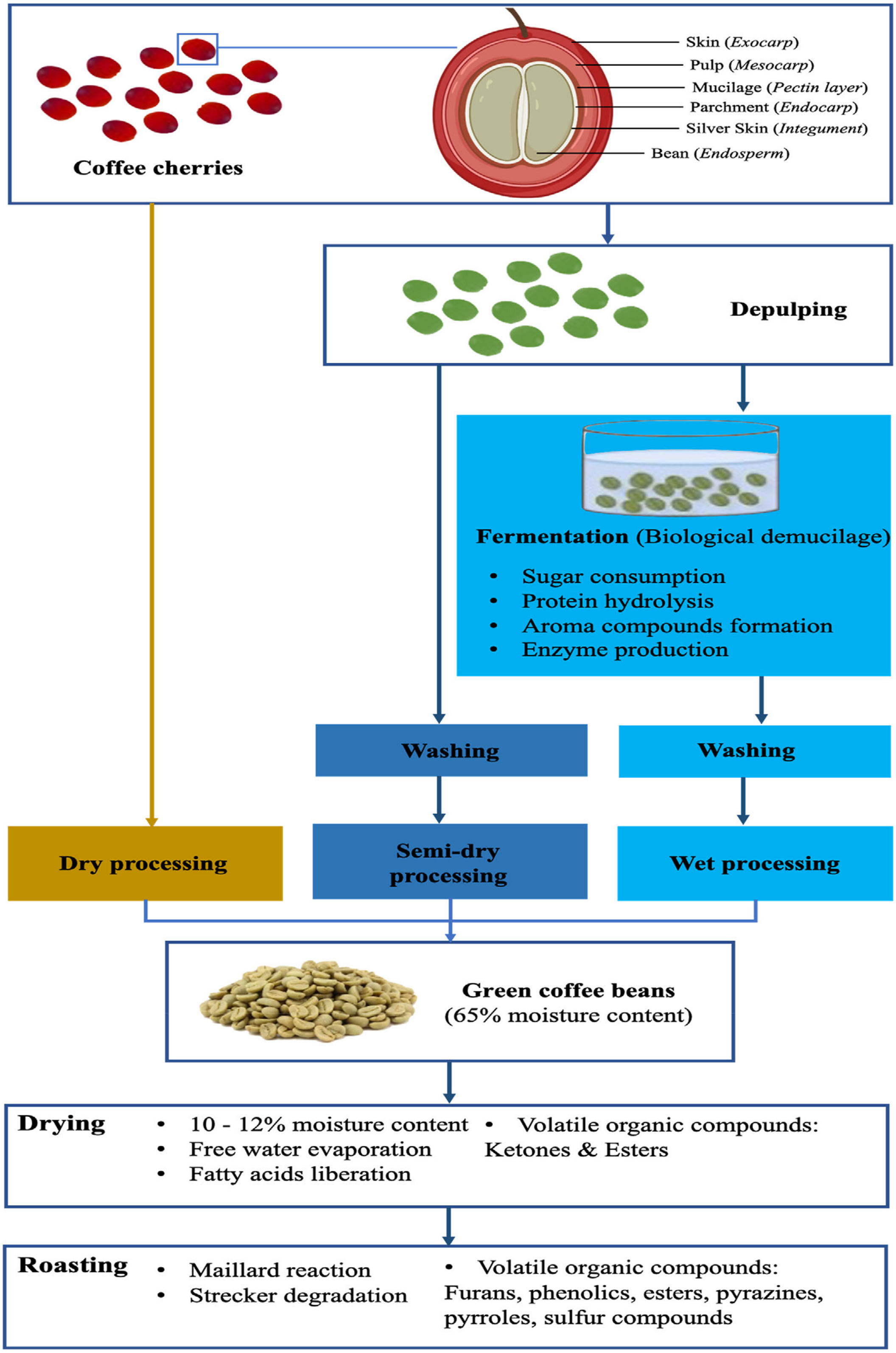


Figure 1 Illustration of three post-harvesting processing of coffee cherries.

silver skin is also abundant in polysaccharides and monosaccharides, proteins, polyphenols and other minor compounds (Janissen & Huynh, 2018; de Melo Pereira *et al*., 2019).

The coffee supply chain starts with coffee cherry harvesting by handpicking or mechanical stripping (de Melo Pereira *et al*., 2019). Proper maturity guarantees raw coffee beans not only an ideal content of desirable VOCs but also a reduced phenolic concentration, which could lower the unwanted astringency and improve the organoleptic quality of final products (Viejo *et al*., 2020). The slight environment and practising changes, including the climate, humidity, temperature and manufacturing, would significantly affect the composition and quality of roasted coffee beans from different batches. Therefore, the postharvest processing of coffee beans is supposed to be conducted immediately to avoid unwanted germination, indigenous fermentation and mould generation (de Melo Pereira *et al*., 2019). Simple washing, separating and sorting needs to be conducted primarily to remove the impurities (dust, stone, *etc*.) and defective beans. Subsequently, selected beans will be processed in different procedures (dry, semi-dry and wet processing) to achieve the optimal chemical composition (moisture, sugars, lipids, *etc*.) according to additional quality requirements and thus preserve coffee profitability. Conventional (dry, honey and wet) processing of coffee cherries processing and novel processing (carbonic maceration) could critically influence the pathway and degree of de-pulping and de-mucilage, which is discussed in detail in the following content (de Melo Pereira *et al*., 2019; Junior *et al*., 2021). Those modifications can trigger and regulate the chemical and microbiological fermentation of beans before roasting, producing aromatic precursors (de Melo Pereira *et al*., 2019). Stronger off-aromas were found in green coffee with incomplete mucilage removal than those with entirely de-mucilage, probably because of the unwanted spontaneous fermentation, which could induce the generation of unwanted substances during roasting (Gonzalez-Rios *et al*., 2007a, 2007b). However, since the microflora population present in coffee is dense and diverse, the fermentation could be inconsistent and unpredictable, which remains to be less elucidated.

Natural/dry processing

Natural processing is commonly used in the regions with limited access to water, such as Ethiopia and Brazil (de Melo Pereira *et al*., 2019), where the intact coffee cherries (with mucilage) are dried by sunshine after washing and de-pulping. It depends more on the regional climate, including rainfall (humidity), temperature and atmospheric conditions (Toledo *et al*., 2016). With the mucilage intact, the natural process gives the roasted coffee a rich body and sweet characteristic since abundant polysaccharides and minerals in mucilage, which are the essential precursors of mostly VOCs. The quality of final coffee products may not be uniform because of the dependence on weather factors such as rainfall, sunlight exposure time and temperature. One of the corrective actions conducted by the coffee farmers in Vietnam is to exclusively pick ripe fruits (up to 98%) and process them in a fast and meticulous way, leading to higher coffee quality and stability (Le *et al*., 2020).

Washed/wet processing

Soaking in water is aimed to remove all soft fruit residue of the coffee cherry. The wet environment facilitates microorganism growth and fermentation, especially lactic acid bacteria (LAB), such as *Leuconostoc mesenteroides*, *Lactobacillus plantarum* and *Lb. brevis*, yeasts (*e.g*., *Pichia guilliermondii*, *P. anomala Kluvyeromyces marxianus* and *Saccharomyces cerevisiae*) and mould (Vilela *et al*., 2010; Evangelista *et al*., 2014; de Melo Pereira *et al*., 2019). Water addition could increase the richness and community of bacteria and fungi (da Silva *et al*., 2022). Using specific microorganisms such as *Saccharomyces cerevisiae* and *Lactobacillus rhamnosus* under controlled conditions is a vital regulator in coffee quality improvement *via* microbial process (da Silva *et al*., 2022; Krajangsang *et al*., 2022). Washed coffee tends to have a cleaner and fruity aroma than natural ones. The reasons can be (1) less sugar (fructose and glucose) metabolism involved due to the wet anoxic environment and the removal of fruit pulp and skin; (2) higher content of free amino acids because of the increased protein hydrolysis (Gonzalez-Rios *et al*., 2007b; de Melo Pereira *et al*., 2019). Although the wet process might contribute to the VOCs quantity in the final coffee due to higher microbial diversity, the washed process faces a higher uncertainty on the VOCs quality because of the unknown microbial activity and uncontrolled endpoint, which can cause either a positive or negative impact on the final cup quality (de Melo Pereira *et al*., 2019). Excessive defective VOCs, such as sulphur and phenolic compounds, aminobutyric acid and acetic acid, can be generated if overfermentation due to prolonged exposure to drought stress, which may induce unfavourable bitterness or sourness in the final coffee brew (Toledo *et al*., 2016; de Melo Pereira *et al*., 2019). Recently, the standardisation of fermentation by selecting microbial strains has been highlighted to solve this problem while the operational feasibility remains consideration due to the complicated microbial metabolites (Zhang *et al*., 2019). Besides, proper waste treatment access to sustain the ecosystem around coffee plants is necessary for farmers with mostly wet-processed coffee production fields (Nguyen & Sarker, 2018).

Honey processing

Honey processing combines wet and dry processing, removing the pulp but keeping mucilage before drying. Thus, impurities from pulp could be avoided and potentially allows the well-controlled fermentation of the mucilage around the coffee seeds (de Melo Pereira *et al*., 2019). The glucose and fructose contents in the semi-dried coffee beans were found in between wet (lowest) and dry (highest) processed coffee beans (de Melo Pereira *et al*., 2019). Semi-dry processed coffee bean was reported with higher concentrations of TBARS (thiobarbituric acid reactive substances), which indicated higher lipid oxidation. Additionally, semi-dried coffee beans would show a higher intensity of ‘rested coffee flavour’, defined as a woody taste and pale flavour notes, after 15-month-storage (Rendón *et al*., 2014). Based on the degree of mucilage removal, the semi-drying/honey process can be divided into subclasses: white honey process (80–100% mucilage removal), yellow honey process (50–75% mucilage removal), red honey process (0–50% mucilage removal) and black honey process (the least amount of mucilage removal). The honey process includes moderate water usage and retains a certain level of sweetness and cleanness (Toledo *et al*., 2016). As a combined method compromising between washed and dry processes, both benefits and limitations of these two methods should be considered in the honey process.

Novel technique - carbonic maceration

The carbonic maceration (CM) technology was initially used in the wine-making industry to upgrade the aroma and body and save processing time. It was introduced to the coffee industry recently and is designed to leave the intact coffee beans sealed in an enclosed environment, with expelled O_2 and filled with CO_2. It aims to switch aerobic respiration to anaerobic respiration, encouraging microbial fermentation within the fruits (González-Arenzana *et al*., 2020; Junior *et al*., 2021). Although this method has been rapidly developed, few scientific studies have been published, and it remains an ‘experimental processing method’. Only one study has evaluated the possibility of the CM application in coffee postharvest processing (Junior *et al*., 2021). The authors observed a significant impact of the CM method on the sensorial, chemical and microbiological profiles of their *Arabia* coffee sample. However, this area remains further elucidated.

Chemical reactions during coffee roasting

Coffee roasting is a complex thermal process, including colour browning, moisture reduction (from 10% to 30%) and structural porosity improvement. Numerous VOCs could be generated *via* multiple chemical reactions, which are essential to the coffee aroma (Ruosi *et al*., 2012). Zakidou *et al*. (2021) found a total of 138 VOCs in 10 types of roasted coffee formed mostly by Maillard reactions (30–40%), followed by Strecker degradation (16–18%), and other responses (30–37%) (pyrolysis and fragmentation). Around 300 VOCs have been found in raw coffee beans, while over 850 in roasted coffee, which determines the final cup profile (Flament, 2001).

Roasting conditions significantly impact those chemical changes, VOCs yields and sensory quality. Gonzalez-Rios *et al*. (2007b) found that light-roasted (240 °C for 6 min) coffee had the lowest concentration of total VOCs among the three roasting degrees, compared to the medium and dark roasting, which was 240 °C for 7 and 9 min, respectively. Poor-controlled roasting can also cause the further degradation of some desirable VOCs and encourage the formation of undesirable compounds because of intensive pyrolytic reactions (Toledo *et al*., 2016). Ethyl acetate and methyl acetate with fruity, wine-like, grape-like notes and ethanol with a sweet note, could be reduced when the roasting degree increases. Meanwhile, pyridine (sour and fishy notes) would be raised (Moon & Shibamoto, 2009).

Maillard reaction and Strecker degradation

Maillard reaction

During roasting, the Maillard reaction (non-enzymatic browning) could occur when the temperature reaches 140 °C, where carbohydrates and amino acids in coffee beans could start a cascade of reactions along with the development of many aroma-related compounds. As shown in Fig. 2, three stages are involved: (1) the reactions between reducing sugar and amino acids, generating N-substituted glycosylamine and water; (2) the Amadori rearrangement (isomerisation) of the glycosylamine produced in the first step, generating ketoamines (Amadori product); (3) the ketoamines conversion *via* several pathways into fission products and reductones (under alkaline condition), hydroxymethylfurfural (under acidic condition) and melanoidins (brown pigments) (Moreira *et al*., 2012; de Oliveira *et al*., 2016).

Temperature, humidity, pH, the presence of certain metals, and the contents of reducing sugar could affect Maillard reactions (Toledo *et al*., 2016). A wide range of VOCs, including furans, pyrazines and pyrroles, would be generated and contribute to the various coffee aromas (roasted, malty, nutty, bitter and burnt

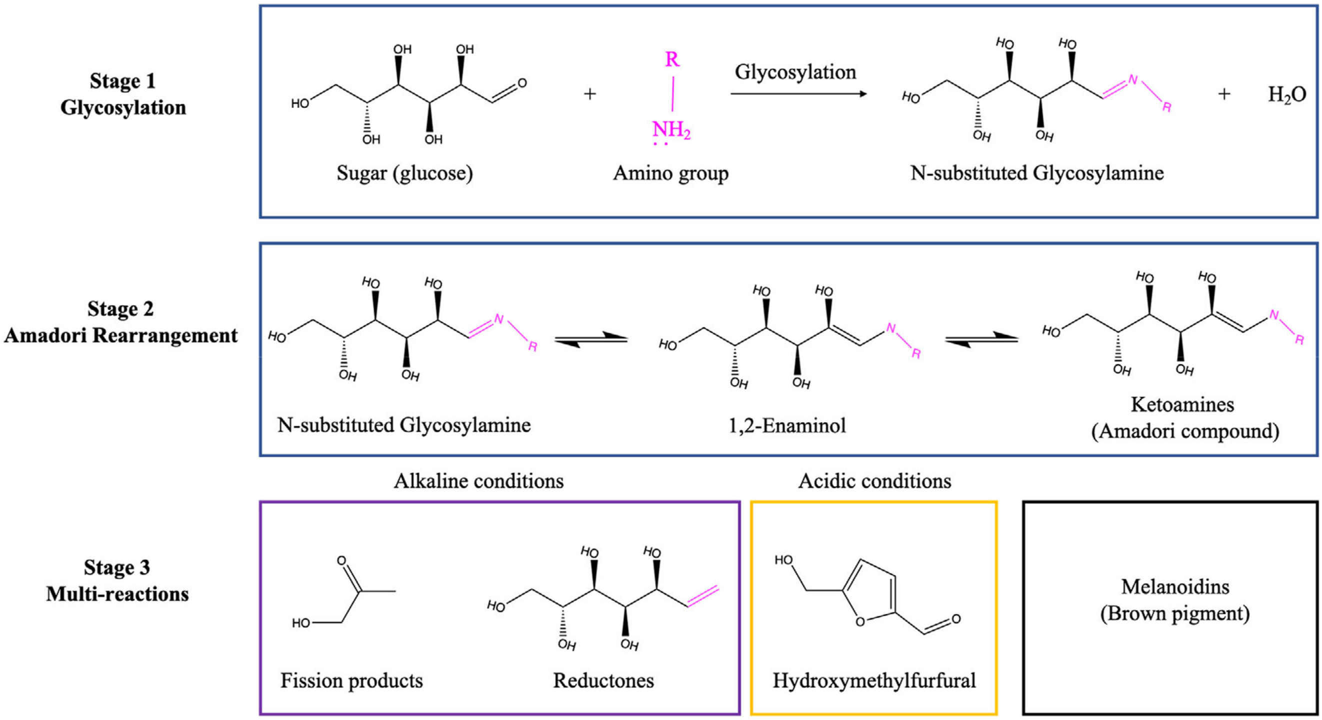


Figure 2 Three stages of Maillard reaction.

aromas) with a significant impact on its sensory quality (Moreira *et al*., 2012). A higher roasting degree could strengthen Maillard reactions and eventually contribute to a higher yield of pyridines and pyrroles, leaving dark-roasted coffee with a chocolate-like and nutty flavour (Moon & Shibamoto, 2009). N-methylpyridine concentration could also start to build up and show an increasing trend from the medium roasting level and reach the highest level at the dark roasting point (Hu *et al*., 2020). Furfural and derivatives (sweet and caramel-like) are found at a relatively higher level in mild-roasted coffee but with a decrease in their higher-roasted counterparts (Moreira *et al*., 2012). Poor Maillard reactions may also cause inadequate generation of VOCs, especially those with nutty, coconut- and chocolate-like features, thus lowering the roasted coffee (Velásquez *et al*., 2019).

Strecker degradation

Strecker degradation is considered a subset of Maillard reactions because of the close linkage. Some of the carbonyl derivatives generated from the Maillard reaction may participate in Strecker degradation with free amino acids, the building blocks of proteins in coffee beans. Two steps are involved: (1) the oxidisation between amino acids (reductant) and carbonyl derivatives (oxidant), and (2) the break-down of the resulting molecules into aldehydes, ammonia and carbon dioxide in the presence of water (Toledo *et al*., 2016). The aldehyde group (acetaldehyde and hexanal) is a crucial part of coffee aroma, which gives coffee a fruity fragrance and indicates coffee freshness (Buffo & Cardelli-Freire, 2004). Besides, the CO_2 created in Strecker degradation can increase the internal pressure, expand beans, make them crack fields and further assist the volatilisation of coffee aroma (Wang & Lim, 2014; Toledo *et al*., 2016).

Caramelisation

Similarly, caramelisation is also a non-enzymatic browning, while it occurs in the absence of amino acids at a relatively higher temperature. As shown in Fig. 3, it focuses on the thermal decomposition of more complex carbohydrates (such as sucrose) in coffee beans into smaller sugar molecules (fructose and glucose) with higher water-solubility at a temperature around 170 °C (Knopp *et al*., 2006). The loss of water molecules from individual sugars is also known as a condensation step. Subsequently, maltol with a caramel taste, acetic acid with sourness and furans with nutty notes could be produced, resulting in a complicated coffee flavour (Knopp *et al*., 2006). Therefore, this step is one of the primary sources of sweet, caramel and almond-like aroma, which could improve the perceived sweetness of final brewed coffee.

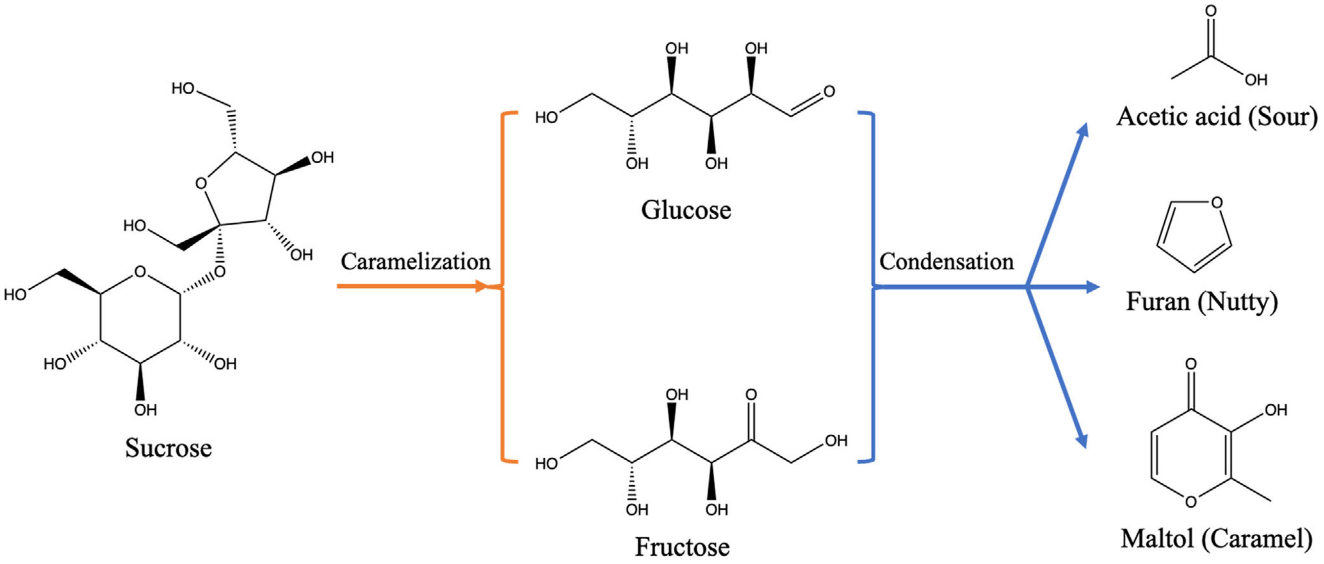


Figure 3 The caramelisation of sucrose during coffee roasting.

Pyrolysis

Pyrolysis reactions happen once the beans are heated to 190 °C. Sucrose pyrolysis can lead to caramelisation, which darkens the bean's colour and produce volatile carbocyclic compounds at 190–200 °C (Montavon *et al.*, 2003). Roasting can cause 3-methylbutanoyl disaccharides (3MDs) pyrolysis in coffee. The products mainly consist of a 3-methylbutanoic acid, which may enhance the richness of coffee flavour (Iwasa *et al.*, 2015; Iwasa *et al.*, 2021). Protein also undergoes pyrolysis and releases aromatic compounds such as alanine and asparagine (Dong *et al.*, 2015). Importantly, coffee lipids/oils pyrolysis can provide strong coffee flavour and antioxidant ability as a functional food and beverage (Vila *et al.*, 2005; Ferrari *et al.*, 2010). The lipid fraction in coffee beans, located in the endosperm, is primarily composed of triacylglycerol, sterols, coffeadiol, arabitol and tocopherols (de Melo Pereira *et al.*, 2019). Although those compounds are found in small thresholds, they can influence central carbon and nitrogen metabolism. Thermal roasting can lead to the self-oxidation of triacylglycerol and lipids, producing alcohols and ketones. Besides, the condensation between fatty acids and alcohol molecules can generate many esters, which have a pivotal role in fruity and flower-like notes in the coffee sensory (de Melo Pereira *et al.*, 2019). Roasting does not trigger dramatic changes in coffee lipid fraction, which may be related to the presence of lipid-soluble products from the Maillard reactions (Amarowicz, 2009), while the roasting conditions can influence the lipid pyrolysis progress. The total polyunsaturated fatty acids (PUFA) content was found to be the highest (45.5%) under roasting at 210 °C with high moisture of heating air among all conditions applied (Budryn *et al.*, 2012).

Other reactions

Based on sugars, dehydration, decarboxylation, fractionation, isomerisation and polymerisation of carbohydrates, are also believed to contribute to coffee flavour development (Wu *et al.*, 2021). During roasting, aroma-related reactions are not only based on sugars and lipids in the coffee matrix but also on protein molecules, such as loss of protein nitrogen, denaturation of protein and degradation of specific amino acids (proline and hydroxy amino acids), which may lead to undesirable sulphur compounds with cabbage- or onion-flavour in the final product. Trigonelline, for instance, is an essential flavour precursor and its degradation products cover a range of pyridine and pyrroles (Montavon *et al.*, 2003). Other nitrogen-containing compounds such as alkaloids and volatile acids (acetic, butanoic and propanoic acids) are also detected in high amounts in green coffee beans, which will be decomposed during roasting and produce influential sensory metabolites (pyridines and pyrroles) (Sunarharum *et al.*, 2014).

Major volatile compounds in roasted coffee

Furans

The most volatile compound contributing to the coffee flavour is furan derivatives (25–41%) with sweet, bread-like and caramel aromas, especially 5-methylfurfural,

furfural and 2-furanmethanol (Flament, 2001; Moon & Shibamoto, 2009). It could be generated by Maillard reactions, caramelisation and thermal-oxidative degradation of the polyunsaturated fatty acids (Moreira *et al.*, 2012; Zakidou *et al.*, 2021). Therefore, the washed coffee generally has a lower content of furans with lower sweetness and chocolate flavour after roasting since the removal of mucilage causes less sugar to be available as substrates for these reactions (Gonzalez-Rios *et al.*, 2007a; Zakidou *et al.*, 2021). 5-Methylfurfural is one of the most important contributors to the desirable caramel aroma of roasted coffee. Wet processing has been confirmed to improve the volatilisation of more 5-methylfurfural in roasted coffee beans due to the mucilage removal (González-Arenzana *et al.*, 2020). Besides, furan and derivatives are the most influenced by burning conditions, especially 5-hydroxymethylfurfural significantly, which decreased from 26.8% (230 °C 12 min) to 0% (250 °C 21 min) and furfural from 19.9% to 2% (Moon & Shibamoto, 2009). This decrease may result from VOCs' more significant decomposition and polymerisation as roasting degrees rise. However, other furans identified in coffee and formed during roasting, such as 3-Methylfuran are considered potentially carcinogenic and toxic and are still under investigation by the International Agency for Research on Cancer (IARC) (Becalski *et al.*, 2016; Rahn & Yeretzian, 2019; Gonzalez Viejo *et al.*, 2021b).

Pyrazines

Pyrazines are the second most abundant VOCs (25–39%) in roasted coffee generated through complex sugar-amino-acid interactions, known for their hazelnut aroma in the coffee brew (Zakidou *et al.*, 2021). 2-Ethyl-3,5-dimethylpyrazine, 2,6-dimethylpyrazine, 2-ethyl-6-methyl pyrazine and 2-ethyl-3,5-dimethylpyrazine have been confirmed as the potent odorants in the final products (Toci & Farah, 2014). Under the same roasting conditions, a drier postharvest process gives higher pyrazine formation after coffee roasting along with a more robust hazelnut flavour (Gonzalez-Rios *et al.*, 2007a; Hameed *et al.*, 2018).

Aldehydes

Aldehydes, formed *via* Strecker degradation, are highly aromatic compounds that contribute to the spectrum of coffee aromas, including chocolate-like, floral, honey-like, fruity, roasting and earthy (Gigl *et al.*, 2021). For example, phenylacetaldehyde has a floral and honey-like aroma; methylbutanal is usually perceived as malty or chocolate-like, while propanal and hexanal obtain fruity and green odour (Flament, 2001; Barrios-Rodríguez *et al.*, 2021). The postharvest process influences the generation and extraction of aldehydes. Compared to the wet process, the dry process gives coffee a relatively higher aldehyde content, with a more pungent fruity/wine-like taste and heavier body in the coffee brew, where the different aldehydes may be generated from mucilage remnants (Hameed *et al.*, 2018). However, a drop in 3-methylbutanal and 2-phenylethanal (malty aroma) could be observed after proteolytic and lipolytic yeast fermentation (Lee *et al.*, 2017a, 2017b). Furthermore, aldehydes tend to be influenced more readily by other VOCs. A strong positive correlation ($r = 0.752$, $P < 0.001$) between aldehyde and ketone groups but negative correlations with pyrazines and phenols were observed (Caporaso *et al.*, 2018). Similarly, Zakidou *et al.* (2021) also found that aldehydes and ketones corporately contributed to 1–6% of the VOCs in coffee, while none of the other single compounds was more than 1%. Thus, aldehydes can be generated *via* the oxidation of amino acids and polyphenols when polyphenol oxidase is present (Caporaso *et al.*, 2018).

Ketones

Ketones are initially found in raw coffee beans as the products of oxidative degradation of fatty acids. During roasting, the main pathway of ketone formation includes Maillard reactions, caramelisation, alcohol oxidation and auto-oxidation of unsaturated fatty acids (Flament, 2001). In this class, the potential coffee-odorant compounds contributing to creamy, buttery and caramel flavour notes include acetoin, 2,3-pentanedione, β-Damascenone, 1-hydroxy-2-propanone, 1-hydroxy-2-butanone and 2,3-butanedione (Ribeiro *et al.*, 2018; de Melo Pereira *et al.*, 2019). Besides, the variability of single-origin coffee VOCs and reported ketones as the most uniform VOCs with a coefficient of variation (CV) < 20% (Caporaso *et al.*, 2014). Roasting speed also affects the performance of ketone formation. Slow and medium roasting can give rise to a higher level of ketones in roasted coffee (Hameed *et al.*, 2018). However, over-fermentation caused by improper postharvest processing (such as uncontrolled microbial growth or over-dense drying area >20 kg m^{-2}) could result in a foul smell and undesirable taste in the final cup. Among these defective/degraded compounds, ketones are one of the most significant off-flavour makers (Toci & Farah, 2014).

Phenolic compounds

In the category of phenols/phenolic compounds, guaiacol, 4-vinylguaiacol and 4-ethylguaiacol are the primary aromatic contributors in roasted coffee, bringing a well-documented spicy and smoky note (Piccone *et al.*, 2012; de Melo Pereira *et al.*, 2019; Zakidou *et al.*, 2021). Although roasting determinately regulates phenol productions because phenols are mainly generated from the thermal degradation of chlorogenic acids and the decarboxylation of carboxylic acids, other postharvest processing also influences the coffee phenols formation (Zakidou *et al.*, 2021). Phenols are found in higher concentrations in higher/darker roasting-intensity coffee (Moon & Shibamoto, 2009; Gonzalez Viejo *et al.*, 2021b). The contents of volatile phenols, including 4-methoxyphenol, 4-ethylguaiacol and 4-vinylguaiacol, were the topmost in washed coffee but decreased in the semi-wet process and dry process (Toledo *et al.*, 2016). Furthermore, all aroma-related phenols were detected in roasted coffee, while not all exist in green beans (Lee *et al.*, 2017a, 2017b; de Melo Pereira *et al.*, 2019). Notably, the flavour contributions of phenols may differ in different concentrations, as guaiacol tends to have a burnt flavour at a relatively higher concentration while sweet at a lower concentration (Gonzalez-Rios *et al.*, 2007b; González-Arenzana *et al.*, 2020). Besides, phenol contents were observed with a higher intra-batch variation (above 40% CV), even representing over 100% CV in some coffee samples (Caporaso *et al.*, 2018).

Sulphur compounds

Sulphur compounds are mainly produced during thermal roasting and lead to an undesirable vegetable, putrid and garlic smell even at a low threshold, which shows an unignorable effect on the human olfactory perception (Dulsat-Serra *et al.*, 2016). For example, methanethiol is described with cabbage and rotten egg smell and is considered an indicator of low-quality coffee, especially 3-methyl-2-buten-1-thiol (amine-like contributor) (Caporaso *et al.*, 2018; De Melo Pereira *et al.*, 2020, 2019; Zakidou *et al.*, 2021). The widely accepted formation of sulphur compounds is the interactions among sulphur-containing amino acids, sugars and other minor chemicals. Maillard reactions largely account for thiols generations while pentoses- or hexoses-cysteine reactions for 2-furfurylthiol and 2-methyl-3-furanthiol (Dulsat-Serra *et al.*, 2016). Thus, the roasting process is more influential on coffee thiol production than other postharvest processes.

Volatile acids and fatty acids

Acids produced *via* microbial fermentation during coffee processing may induce a pungent and sour flavour; however, it could enhance the complexity of coffee flavour and bring a rounder cup taste with a small amount (Bressani *et al.*, 2020). For example, acetic acid (a simple monocarboxylic acid) could bring a taste of vinegar on its own but can contribute to a wine-like and sweet flavour paired with other compounds while a saturated short-chain fatty acid, isovaleric acid (3-methylbutanoic acid), with cheese-like rancidity was also identified as a potential odorant in brewed coffee (Chin et al., 2011). Besides, quantitative analysis confirmed isovaleric acid as an indicator of excellent coffee quality, over 80 scored by Speciality Coffee Association (SCA) (Iwasa *et al.*, 2021). Fatty acid (FAs) fractions of triacylglycerols have a subtle but desirable flavour note in coffee. It has also been proven beneficial to human health due to its precursor role of eicosanoid production, a bioregulator of many cellular metabolisms (Dong *et al.*, 2015). Linoleic acid (C18:2) is an essential polyunsaturated fatty acid that requires humans from external sources and is found in large amounts in roasted coffee Fields (Couto *et al.*, 2009). In addition, palmitic acid (C16:0) and archaic acid (C20:0) are the primary saturated fatty acids, while oleic acid (C18:1) is the monounsaturated fatty acid present in the roasted coffee (Wagemaker *et al.*, 2011; Dong *et al.*, 2015) (Table 1).

Other VOCs

Other VOCs, including esters, pyrroles, pyridines and alcohol, are also found in roasted coffee and affect coffee sensory quality. Pyrrole derivatives are a subsidiary class of VOCs found in the coffee brew (5–12%), particularly 1-methyl-1H-pyrrole-2-carboxaldehyde, 2-acetylpyrrole and 2-formylpyrrole, contributing roasted, nutty and cocoa notes (Zakidou *et al.*, 2021). They could be generated during the thermal degradation of Amodori intermediates, caramelisation, pyrolysis and trigonelline degradation (Flament, 2001; Zakidou *et al.*, 2021). Ester group represents the third abundant in roasted coffee (5–8%) by two major compounds, 2-furan methanol acetate (3.7–5.8%) and propanoate (around 1.3%), which develop the fruity aroma (Zakidou *et al.*, 2021). Gonzalez Viejo *et al.* (2021b) found 2-furan methanol acetate as the most abundant VOC in Nespresso® coffee pods with different roasting intensities and reported related aromas such as fruity, banana, floral and ethereal. Likewise, fermentation favours coffee esters formation leading to a higher concentration of ethyl acetate, methyl acetate and ethyl isovalerate. Ethanol and 2-phenyl ethanol from the alcohol class has a sweet and floral aroma. Pyridines could be generated through the thermal degradation of Amodori intermediates and pyrolysis of amino acids and trigonelline, contributing 3–6% presence in roasted coffee. However, different postharvest practices could also randomly alter the pyridine formation (Flament, 2001).

Coffee sensory

Coffee provides a diverse sensory experience, including aroma, taste, mouthfeel and aftertaste. Among these,

Table 1 Common VOCs in roasted coffee with molecular formula, chemical structure and description notes; all molecular formula and chemical structure are cited from PubChem

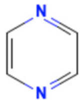
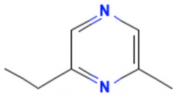
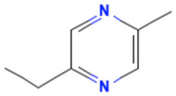
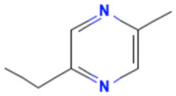
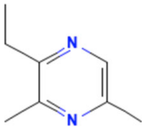
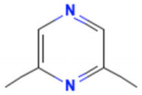
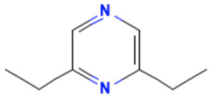
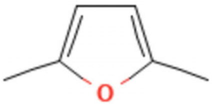
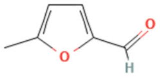
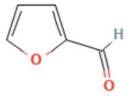
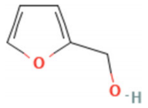
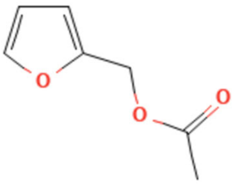
Compound classification	Compound name	Molecular formula	Chemical structure	Aroma notes	References
Pyrazines	Pyrazine	$C_4H_4N_2$		Nutty, roasted, pungent	De Melo Pereira *et al.* (2019), Zakidou *et al.* (2021)
	2-Ethyl-6-methylpyrazine	$C_7H_{10}N_2$		Cocoa, roasted, hazelnut-like	Akiyama *et al.* (2003), Zakidou *et al.* (2021)
	2-Ethyl-5-methylpyrazine	$C_7H_{10}N_2$		Nutty, coffee-like	Caporaso *et al.* (2014), Zakidou *et al.* (2021)
	2,6-Dimethylpyrazine	$C_6H_8N_2$		Nutty, cocoa, coffee-like	Zakidou *et al.* (2021)
	2-Ethyl-3,5-dimethylpyrazine	$C_8H_{12}N_2$		Nutty, burnt, almond-like, roasted	de Melo Pereira *et al.* (2019), de Morais *et al.*, 2007, Zakidou *et al.* (2021)
	2,6-Diethylpyrazine	$C_6H_8N_2$		Nutty, toasted	Gonzalez-Rios *et al.* (2007b), Caporaso *et al.* (2018)
	2,6-Dimethylpyrazine	$C_8H_{12}N_2$		Nutty, roasted, cocoa-like, coffee-like	Zakidou *et al.* (2021)
Furans	2,5-Dimethylfuran	C_6H_8O		Meaty, roasted, ethereal; coffee-like	Flament (2001), Gonzalez-Rios *et al.* (2007b), Alstrup *et al.* (2020), Zakidou *et al.* (2021)
	5-Methylfurfural	$C_6H_6O_2$		Caramel, maple, spicy, sweet	de Melo Pereira *et al.* (2019), Zakidou *et al.* (2021)
	furfural	$C_5H_4O_2$ or C_4H_3OCHO		Sweet, woody, almond-like	Gonzalez-Rios *et al.* (2007b), Zakidou *et al.* (2021)
	2-Furanmethanol	$C_5H_6O_2$		Caramel, warm-oily, burnt, smoky	Flament (2001), Zakidou *et al.* (2021)
	Furfuryl acetate	$C_7H_8O_3$		Sweet, fruity, banana	(Evangelista *et al.* (2015), Yanagimoto *et al.* (2002)

Table 1 (*Continued*)

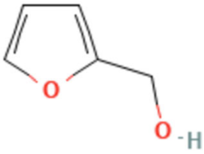
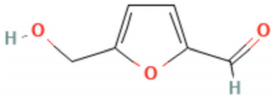
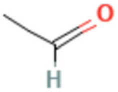
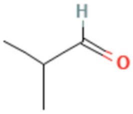
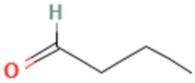
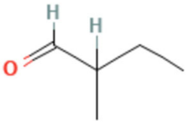
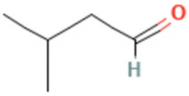
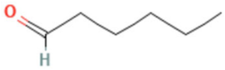
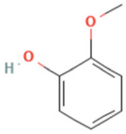
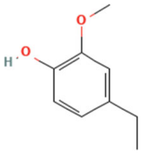
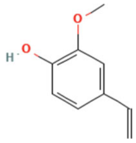
Compound classification	Compound name	Molecular formula	Chemical structure	Aroma notes	References
	Furfuryl alcohol	$C_5H_6O_2$		Sweet, caramel, brown sugar	Evangelista *et al.* (2015), Poyraz *et al.* (2016)
	5-Hydroxymethylfurfural	$C_6H_6O_3$		Buttery, caramel	Zakidou *et al.* (2021)
Aldehydes	Acetaldehyde	C_2H_3O		Fruity, fresh, green	Caporaso *et al.* (2018), de Melo Pereira *et al.* (2019), Zakidou *et al.* (2021)
	2-Methylpropanal	C_4H_8O or $(CH_3)_2CHCHO$		Fruity, malty,	Caporaso *et al.* (2014)
	Butanal	C_4H_8O or $CH_3CH_2CH_2CHO$		Fruity, chocolate	Caporaso *et al.* (2018), López-Galilea *et al.* (2006)
	2-Methylbutanal	$C_5H_{10}O$		Fruity, malty, roasted cocoa, musty	Caporaso *et al.* (2014)
	3-Methylbutanal	$C_5H_{10}O$		Fruity, malty, peach, cocoa	Flament (2001), Caporaso *et al.* (2014), de Melo Pereira *et al.* (2019)
	Hexanal	$C_6H_{12}O$		Fruity, leafy, fatty, grassy	Flament (2001), Caporaso *et al.* (2014), Zakidou *et al.* (2021)
Phenols	Guaiacol	$C_7H_8O_2$		Smoky, spicy, burnt,	Schenker *et al.* (2002)
	4-Ethylguaiacol	$C_9H_{12}O_2$		Smoky, spicy, roasted	Gonzalez-Rios *et al.* (2007b), de Melo Pereira *et al.* (2019)
	4-Vinylguaiacol	$C_9H_{10}O_2$		Smoky, spicy, clove-like	Flament (2001), Caporaso *et al.* (2014), Zakidou *et al.* (2021)

Table 1 (*Continued*)

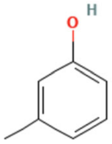
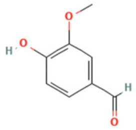
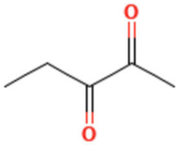
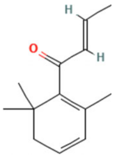
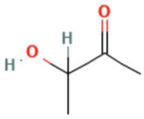
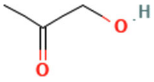
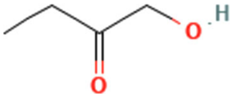
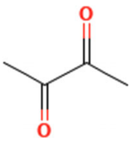
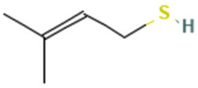
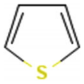
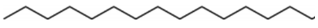
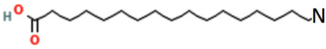
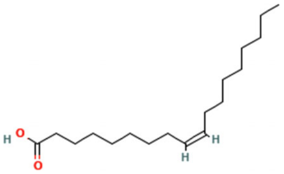
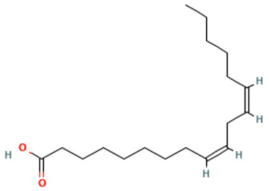
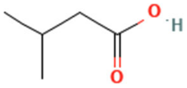
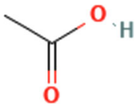
Compound classification	Compound name	Molecular formula	Chemical structure	Aroma notes	References
	3-Methylphenol	C_7H_8O		Woody, leather-like	Lee *et al.* (2017a, 2017b), de Melo Pereira *et al.* (2019)
	Vanillin	$C_8H_8O_3$		Vanilla, sweet	Schenker *et al.* (2002), Zakidou *et al.* (2021)
Ketones	2,3-Pentanedione	$C_5H_8O_2$		Buttery, oily-like, caramel	Caporaso *et al.* (2014), López-Galilea *et al.* (2006), Zakidou *et al.* (2021)
	β-Damascenone	$C_{13}H1_8O$		Floral, fruity, honey-like	Caporaso *et al.* (2014), Schenker *et al.* (2002)
	Acetoin	$C_4H_8O_2$		Buttery, creamy, dairy-like	de Melo Pereira *et al.* (2019), Zakidou *et al.* (2021)
	1-Hydroxy-2-propanone	$C_3H_6O_2$		Sweet, caramel	Zakidou *et al.* (2021)
	1-Hydroxy-2-butanone	$C_4H_8O_2$		Sweet, caramel	Gonzalez-Rios *et al.* (2007b), de Melo Pereira *et al.* (2019), Zakidou *et al.* (2021)
	2,3-Butanedione	$C_4H_6O_2$		Buttery, creamy, caramel	de Melo Pereira *et al.* (2019), Evangelista *et al.* (2015)
Sulphur compounds	Methanethiol	CH_4S		Cabbage-like, garlic, rotten egg	Blank *et al.* (1991)
	3-Methyl-2-buten-1-thiol	$C_5H_{10}S$		Amine-like	Blank *et al.* (1991)
	Thiophene	C_4H_4S		Sulphur-like, garlic	Zakidou *et al.* (2021)
Fatty acids	Palmitic acid (SFA)	$C_{16}H_{32}O_2$		Cheese-like	Wagemaker *et al.* (2011)
	Arachic acid (SFA)	$C_{20}H_{40}O_2$	 N/A	N/A	Dong *et al.* (2015)

Table 1 (*Continued*)

Compound classification	Compound name	Molecular formula	Chemical structure	Aroma notes	References
	Oleic acid (MUFA)	$C_{18}H_{34}O_2$	 N/A	N/A	Dong *et al.* (2015)
	Linoleic acid (PUFA)	$C_{18}H_{32}O_2$		Vinegar-like	Dong *et al.* (2017)
	Isovaleric acid (SFA)	$C_5H_{10}O_2$		Cheese-like, dairy, rancid	Dong *et al.* (2017), de Melo Pereira *et al.* (2019)
Other organic acids	Acetic acid	$C_2H_4O_2$		Pungent, sour, vinegar-like, fermented	Dong *et al.* (2015), de Melo Pereira *et al.* (2019), Zakidou *et al.* (2021)

MUFA, monosaturated fatty acid; PUFA, polyunsaturated fatty acid; SFA, saturated fatty acid.

the smell and taste of coffee contribute to the overriding understanding of consumption. As shown in Fig. 4, multiple attributes of coffee sensory descriptions are covered and illustrated in detail in the coffee flavour wheel (Bolger *et al.*, 2017).

Contributed by VOCs, the coffee odour is the first descriptor perceived when obtaining the sample beside the visual attributes. Odours are perceived *via* orthonasal, meaning that the volatile compounds travel through the nose to reach the olfactory bulb when sniffing. More complex attributes are the aromas, which are perceived once the product is introduced into the mouth, where the volatile compounds move through the larynx towards the olfactory system (Landis *et al.*, 2005; Small *et al.*, 2005). Concerning humans, the sense of smell is greatly more sensitive than taste. Generally, the smell of ground coffee before pouring water is called fragrance, while the aroma is always referred to as once water is added, regardless of the distinction between the odour and aroma used in sensory and health sciences as described above (Lingle & Menon, 2017). Thus, the term 'aroma' is used in this review because coffee is consumed in liquid. VOCs with different functional groups contribute to the other coffee aromas, influenced by many factors, from the variety of the beans to postharvest treatment. In this case, most light will be shed on the effect of postharvest practices on the VOCs production and thus sensory quality (Zakidou *et al.*, 2021). Most VOCs come from Maillard reactions, Strecker degradation and other heat-related reactions, and thus the VOCs quantity and quality are primarily associated with the roasting process (Zakidou *et al.*, 2021). Common sensory attributes related to coffee flavour include acidity, sweetness and bitterness, all of which are closely associated with the performance of the postharvest process (Alstrup *et al.*, 2020). The dry process typically gives coffee a sweeter taste due to higher fructose and glucose contents which are significantly reduced in washed coffee (de Melo Pereira *et al.*, 2019).

With the help of a humid environment, those sugars as the core reactant substances can promote more robust metabolism and heat-related reactions, producing enjoyable coffee VOCs such as furans and pyrazines. Zakidou *et al.* (2021) investigated ten types of coffee beans and summarised that furan derivatives (5-methyl furfural and 2-furan methanol) were characterised as sweet-like aromas in coffee while pyrazines (2-ethyl-3,5-dimethyl pyrazine) brought nutty and chocolaty flavour. The common VOCs found in roasted coffee with their descriptive notes in previous research are shown in Table 1. The washed process

Figure 4 The coffee tastes and aromas wheel (Bolger *et al*., 2017).

also facilitates the hydrolysis of proteins. Thus, it increases the concentrations of free amino acids in roasted coffee, which is believed to contribute to the fruity taste (de Melo Pereira *et al*., 2019). Well-controlled alcoholic or lactic fermentation may also develop further under wet conditions due to the diversity and community of more microorganisms (Joët *et al*., 2010; de Melo Pereira *et al*., 2019). Like dairy products, where extra-cream milk has a heavier mouthfeel than full-cream and low-fat dairy, coffees can have a similar taste and aroma but a different mouthfeel - trigeminal sensations and flavour (combination of aromas, tastes and mouthfeel). Mouthfeel attributes can be described as thin, heavy/whole, juicy, buttery, creamy or astringent mouthfeel (Hayakawa *et al*., 2010). Two indicators are considered about coffee aftertaste: the lasting time of the taste and whether it is pleasant. Generally, coffee with a prolonged and pleasant aftertaste is the most rewarded. Coffee with an eliminated presence of off-flavour scored higher in clean cup quality, which indicates a proper postharvest treatment such as an efficient sorting step and well-controlled fermentation (Hameed *et al*., 2018).

From the perspective of sensory analysis, Quantitative Descriptive Analysis (QDA®) by the trained panel is commonly used in the production and development of the food and beverage industry. The principle of the QDA® method is to develop a comprehensive and quantitative product description based on the ability of a trained party to quantify specific attributes (Hunaefi *et al*., 2020). It is a widespread tool to quantify descriptors related to the appearance, aroma, texture, mouthfeel, taste and flavour characteristics of brewed coffee (Liseth *et al*., 2019). However, the cost of obtaining professional panellists is relatively high, and the results of this method could be subjective (Kemp *et al*., 2011; Fuentes *et al*., 2018; Fuentes *et al*., 2021b).

Advanced technology in the coffee volatile compounds determination

VOCs analysis – GC-MS

Gas chromatography coupled with mass spectrometry (GC-MS) is a useful tool for VOCs determination in food matrix such as yoghurt, cheese, roasted coffee and wine (Delgado *et al.*, 2010; Piccone *et al.*, 2012; Sunarharum *et al.*, 2014; Caporaso *et al.*, 2018). Along with the GC-MS test, solid-phase microextraction (SPME) is commonly used for the extraction and pre-concentration (using proper absorbing materials to collect the targeted compounds continuously) of the volatile fraction, which is simple, fast and requires minimal treatment and amount of sample, either solid or liquid (Blake *et al.*, 2009; Delgado *et al.*, 2010). The validation of SPME/GC-MS to determine and track the VOCs in roasted coffee is well-documented (De Toledo *et al.*, 2017; De Melo Pereira *et al.*, 2019; Angeloni *et al.*, 2020; Lolli *et al.*, 2020). Zakidou *et al.* (2021) found over 130 compounds in roasted coffee samples through SPME/GC-MS, with an extensive range of chemical categories, including pyrazine, ester furan and pyrrole, among others. SPME/GC-MS was also utilised to compare the odour compounds in Ethiopian coffee and detect 80 VOCs with 14 chemical classes (Akiyama *et al.*, 2005). Also, 81 compounds (of 10 chemical classes) were successfully measured in commercial coffee *via* the GC-MS analysis (Lee *et al.*, 2013b). Over 70 potential odorant compounds were identified by GC-MS in green and roasted ground coffees, with 12 chemical classes (Lee *et al.*, 2017). Besides, numerous studies have also authorised the capability of GC-MS on adulteration in the food industry (Cheong *et al.*, 2013; Peris & Escuder-Gilabert, 2016; Dong *et al.*, 2017). Besides, as a variant of gas chromatography, Proton-transfer Reaction Mass Spectrometry (PTR-MS) is almost exclusively for gaseous compounds detection, making it suitable for coffee VOCs detection, with the advantages of being fast (<1 min) and high detection sensitivity. However, the PTR-MS technique relies on mass spectrometry to discriminate compounds, which may lead to misdetection or identify all the species present when different molecules have the same mass weight present in a complex VOCs mixture (Blake *et al.*, 2009). Hence, applying GC techniques in detecting VOCs shows promise in the coffee area.

E-nose

With the chemical detection of VOCs, sensory analysis of coffee aromas is also conducted in academic studies. Traditional methods such as a descriptive sensory panel or quantitative descriptive analysis (QDA®) are widely used (Dzung *et al.*, 2003). Nonetheless, these techniques employ human perceptions, which may be less reliable when panel members are subjected to biases such as stimulus errors (the assessors make judgements with additional information) and data variance based on panellists (Kemp *et al.*, 2011). Moreover, these methods tend to be time-consuming, expensive and significantly vary between and within individual fields (Gonzalez Viejo *et al.*, 2021b; Fuentes *et al.*, 2021a). A new technique, electronic nose (e-nose), can remarkably save global data and recognise numerous and diverse odorant substances, including aldehydes, pyrazines and ketones, for the chemometric analysis (Pearce *et al.*, 2006; Severini *et al.*, 2015; Dong *et al.*, 2017).

The Digital Agriculture Food and Wine Group from The University of Melbourne (DAFW; UoM) developed a portable and low-cost e-nose composed of an array of nine gas sensors, coupled with machine learning modelling as a rapid method to detect the aromas in food products such as coffee, beer and wine and agricultural applications such as pest detection in wheat (Viejo *et al.*, 2020; Gonzalez Viejo *et al.*, 2021a, 2021b; Summerson *et al.*, 2021a, 2021b; Fuentes *et al.*, 2021c). Fig. 5 illustrates its sample-handling part, featuring a 92-mm-diameter and light-weight system armed with a temperature and humidity sensor

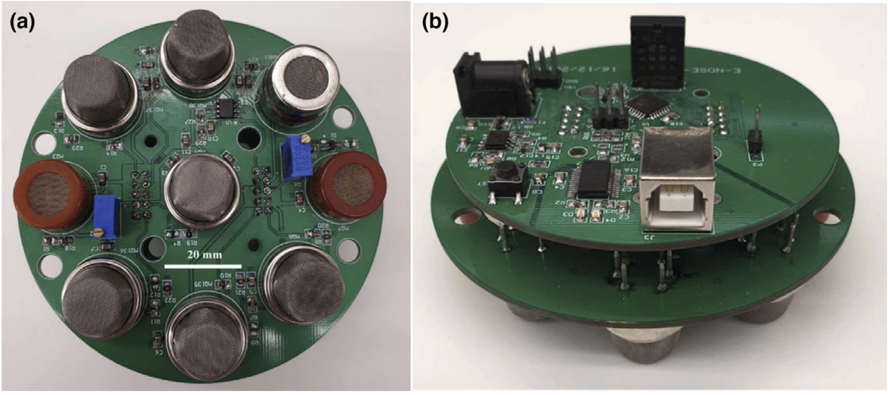


Figure 5 Structures of (a) the portable e-nose system with nine gas sensors (b) stalked multiple printed circuit board (PCB) design to reduce the footprint (Viejo *et al.*, 2020).

Table 2 Specifications of the nine gas sensors and a temperature-humidity sensor for beer characterisation (Henan Hanwei Electronics Co., Ltd), modified from Viejo *et al.* (2020)

Sensor	Measurement	Sensitivity
MQ3	Ethanol	0.05–10 mg L^{-1}
MQ4	Methane	200–10 000 ppm
MQ7	Carbon monoxide	20–2000 ppm
MQ8	Hydrogen	100–10 000 ppm
MQ135	Ammonia alcohol benzene	10–300 ppm; 10–300 ppm; 10–1000 ppm
MQ136	Hydrogen sulphide	1–100 ppm
MQ137	Ammonia	5–200 ppm
MQ138	Benzene alcohol ammonia	10–1000 pp; 10–1000 ppm; 10–3000 ppm
MG811	Carbon dioxide	350–10 000 ppm
AM2320	Humidity temperature	0–99%; 40–80 °C

(AM2320, Guangzhou Aosong Electronics Co., Ltd., Guangzhou, China) aimed to ensure all samples are analysed under similar conditions (ambient and relative humidity). It consists of nine gas sensors, and their specifications are shown in Table 2 (Henan Hanwei Electronics Co., Ltd, Zhengzhou, China) (Fuentes *et al.*, 2020; Gonzalez Viejo & Fuentes, 2020; Viejo *et al.*, 2020). A Microcontroller with an onboard ADC was employed to read the voltages at the interval of 500 ms. In their study, significant differences among aromas in different beers were successfully obtained, which indicated the discriminability of VOCs of e-nose. Furthermore, two highly accurate artificial neural network (ANN) models were developed to predict (i) 17 volatile aromatic compounds with the GC–MS targets (accuracy: $R = 0.97$) and (ii) the intensity of 10 sensory descriptors with sensory targets using QDA® (accuracy: $R = 0.93$). The same research group used the e-nose to assess coffee pods with different roast intensities along with two ANN models to (i) classify samples according to the roast intensity level (accuracy: 98%) and (ii) predict 45 volatile aromatic compounds with GC-MS targets (accuracy: $R = 0.99$) (Gonzalez Viejo *et al.*, 2021b).

Recently, the e-nose has been widely used in many fields (coffee, wine, fish and saffron) to assess the quality of aromatic products due to its rapid, user-friendly and non-invasive nature (Kiani *et al.*, 2016; Marek *et al.*, 2020; Viejo *et al.*, 2020). Marek *et al.*, 2020 utilised e-nose, assisting with GC-MS, to analyse and compare the volatile substances in roasted coffee samples from different countries, proving the suitability for discrimination of coffee aromas. Similarly, Flambeau *et al.* (2017) successfully grouped Rwandan coffee (Bourbon varietal) into sub-regional classes (such as northern and southern areas in Rwanda) based on their aroma profiles *via* e-nose. Furthermore, combined with the electronic tongue (e-tongue) technique, the capability of the e-nose system on coffee physiochemical determination, including pH value, titrate acidity (TA), total solids (TS), total soluble solids (TSS) and TSS/TSA ratio, has been verified in their study of Chinese *Robusta* coffee differentiation (Dong *et al.*, 2017). E-nose is also a valuable tool for determining the optimal time for coffee to be packaged, making a difference in the commercial coffee industry (Falasconi *et al.*, 2003).

Other techniques

Some other techniques in coffee VOCs qualification and quantification in the past few years can be used. For instance, Gas chromatography–olfactory (GC-O) combined with Solid Phase Microextraction (SPME) has attempted the discrimination of coffee beans with the different postharvest processes by integrating the separate VOCs using gas chromatography with an odour detector called olfactometer (human assessor) (Sunarharum *et al.*, 2014). Nuclear Magnetic Resonance (NMR) is another valuable tool to reveal the substantial chemical changes during the coffee postharvest process by detecting the main chemical ingredients in roasted coffee, such as caffeine and caffeoylquinic acids (CQAs) and other water-solvent compounds (Alstrup *et al.*, 2020). Near-Infrared Spectroscopy (NIRS) can monitor the physical changes during coffee processing (moisture, lost weight and density) and perform with high accuracy using iterative predictor weighting (IPW) and partial least square regression (PLS) (Esteban-Díez *et al.*, 2004). To broaden the study scope, more research on those non-volatile compounds that act as precursors in green coffee is required.

Conclusion

The composition of coffee volatile compounds (VOCs) is vital for coffee aroma production. Furans, pyrazines, aldehydes, ketones, phenolic compounds, sulphur compounds, esters, pyrroles, alcohols and pyridines as the influential VOCs found in roasted coffee. Among those, furans and pyrazines are the sweet and hazelnut aroma contributor in roasted coffee, respectively, followed by aldehydes (fruity) and ketones (caramel and buttery), esters (fruity), alcohols (floral and wine-like) and pyridines (chocolate-like) with desirable aroma notes. The degree of off-odours largely depends on the threshold, such as phenolic compounds (roasty and spice-like), pyrroles (cabbage-like) and sulphur compounds (vegetable-like). Microbial fermentation in wet processing could significantly influence the VOC precursor formation and aromatic contribution. Roastingtriggered Maillard reactions, Strecker degradation and caramelisation in coffee beans are the primary reactions related to roasted coffee aroma generation. GC-MS and e-nose sensory analysis are commonly used in coffee quality assurance, with high detectability, accuracy and user-friendly nature. However, novel, low-cost e-noses coupled with machine learning modelling are a portable, reliable and rapid option to assess coffee, especially for small producers in developing countries that cannot afford GC-MS. The variation and interactions among different processing conditions (method, roasting and storage) and numerous unmatured techniques applied in coffee processing still limit further comparison. Thus, future studies need to prioritise those potential barriers to better understand the speciality coffee industry.

Funding information

Dr Hafiz Suleria is the recipient of an “Australian Research Council - Discovery Early Career Award” (ARC-DECRA - DE220100055) funded by the Australian Government. This research was funded by the University of Melbourne under the “McKenzie Fellowship Scheme” (grant no. UoM-18/21) and “Collaborative Research Development Grant (grant no. UoM-21/23)” funded by the Faculty of Veterinary and Agricultural Sciences, the University of Melbourne, Australia.

Conflict of Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Author contributions

Xiaotong Cao: Conceptualization (equal); visualization (equal); writing – original draft (lead). **Hanjing Wu:** Conceptualization (equal); software (equal); visualization (lead); writing – review and editing (lead). **Claudia Gonzalez Viejo:** Investigation (equal); supervision (equal); writing – review and editing (supporting). **Frank R. Dunshea:** Investigation (equal); supervision (equal); writing – review and editing (supporting). **Hafiz A.R. Suleria:** Conceptualization (supporting); data curation (equal); methodology (supporting); supervision (lead); visualization (supporting); writing – review and editing (supporting).

Peer review

The peer review history for this article is available at https://publons.com/publon/10.1111/ijfs.16261.

Acknowledgment

Open access publishing facilitated by The University of Melbourne, as part of the Wiley - The University of Melbourne agreement via the Council of Australian University Librarians.

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