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Extraction kinetics of coffee aroma compounds using a semi-automatic machine: On-line analysis by PTR-ToF-MS

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ABSTRACT

The hot-water extraction process used to make an espresso coffee is affected by a large number of factors. A proper understanding of how these factors impact the profile of the final cup is important to the quality of an espresso coffee. This work examines the effect of water temperature and pressure on the extraction kinetics of volatile organic compounds (VOCs) in coffee. This was achieved by on-line monitoring of the volatiles directly from the coffee flow, using proton-transfer-reaction time-of-flight mass-spectrometry (PTR-ToF-MS). Using hierarchical cluster analysis (HCA), tentatively identified compounds were grouped into 5 families according to their time–intensity profiles. VOCs grouped into each family had similar physicochemical properties while polarity was found to be one of the main forces driving VOC extraction kinetics. The effect of pressure was studied by extracting espresso coffees at 7, 9 and 11 bar. A pressure of 11 bar resulted in an increased extraction of volatiles over the entire extraction time (25 s). To study the effect of temperature, espresso coffees were extracted at 82, 92 and 96 °C. An increase in temperature produced a significant increase in the extraction of VOCs, especially during the last part of the extraction. The effect of temperature on extractability was more pronounced for the less polar compounds.

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1. Introduction

Coffee is one of the most widely consumed beverages [1]. The beverage is made from coffee beans that are first harvested and processed, then roasted and ground before finally being extracted. Each and every single transformation step, from the seed to the cup, must be mastered and performed with great care in order to deliver the best quality in the cup [2–9]. Here, we focused on the last and crucial transformation step, the extraction – more specifically, espresso coffee extraction using a semi-automatic coffee machine.

During extraction, soluble compounds are dissolved and, depending on the extraction technique, non-soluble compounds are washed away with the extraction water, ending up in the extract as dissolved or suspended solids [10–15]. Many different extraction techniques have been introduced over the past centuries, which vary according to factors such as geography, culture and social context, as well as personal preferences; these different factors can result in vastly different flavor profiles in the extract. Of all coffee brewing methods, espresso brewing is among the most popular techniques.

Starting with whole roasted coffee beans, the preparation of the "perfect" espresso is as much a science as an art. It is the result of the interplay between several parameters that must be carefully controlled. These parameters include the particle size distribution of the ground coffee, the water-to-coffee ratio, the final volume of the brew in the cup and the temperature and pressure of the extracting water. An espresso is defined as a 25–35 ml beverage prepared from 7 to 9 g of coffee, through which clean, 92–95 °C water has been forced at 9–10 atmospheres of pressure, and where the grind of the coffee is such that the brewing 'flow' time is approximately 20–30 s [11].

An increase in the extraction temperature, for example, leads to higher quantities of non-volatiles (i.e. total solids, caffeine, lipids) as well as higher quantities of some volatiles, such as pyrazines, in the final cup [16–18]. This may result in over-extraction and a coffee cup with negative flavor notes, such as woody, burnt or acrid flavors. Increasing pressure up to 11 bar also resulted in coffees with higher odor intensity and lower consumer acceptance than coffees

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extracted at 7 or 9 bar [19]. In these previous studies, the authors focused on the composition and sensorial attributes of the final cup in order to assess the impact of water temperature and pressure on espresso preparation. In a complementary line of research, some scientists have been exploring the extraction kinetics of the volatiles that contribute to the aroma of coffee. Two main methods have been previously used to determine the extraction kinetics of coffee volatiles: off-line analysis of fractions using GC–MS [20] and on-line analysis of the volatiles released by the coffee flow using Proton Transfer Reaction Time of Flight Mass Spectrometry (PTR-ToF-MS) [21,22]. In both cases, the methods were applied to single-serve capsule systems in which both temperature and pressure were kept constant. The objective of the research presented here was to investigate the effect of temperature and pressure on the extraction kinetics of coffee aroma compounds by applying on-line analysis by PTR-ToF-MS. We focused on 46 VOCs in particular and explored the link between extraction kinetics and their physicochemical properties.

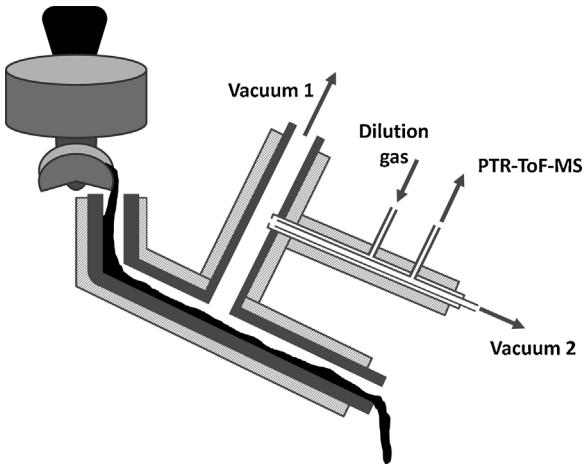

Fig. 1. Setup used for the online monitoring of volatiles during coffee extraction.

2. Materials and methods

2.1. Coffee extraction

The yellow bourbon variety of *Coffea Arabica* L. from Mogiana, Brazil (Roaster: Kaffeepur, Switzerland, "Yellow Sun"), roasted to a medium roast degree of 95 Pt (Colorette 3b, Probat, Germany), was used for all of the extraction experiments. The coffee was frozen two weeks after roasting and defrosted 12 h prior to the experiments to ensure a constant and equal freshness of the coffee for all of the experiments. Less than one month elapsed from roasting to extraction. The beans were ground using a Compak K10 grinder (Barcelona, Spain) using position 47 on a scale from 0 (fine ground, Turkish coffee) to 60 (coarse ground, French Press pot). 18 g of the ground coffee were weighed into a double porta-filter basket, tapered by hand and extracted for 25 s using a semi-automatic coffee machine (Dalla Corte Mini, Dalla Corte, Italy). The water used for the extractions was commercially available Volvic mineral water (total mineralization 130 mg/L; HCO_3^-: 71 mg/L; SO_4^{2-}: 8.1 mg/L; Na^+: 11.6 mg/L; Ca^{2+}: 11.5 mg/L; Mg^{2+}: 8 mg/L). Extractions were performed with five different combinations of water pressure and temperature, one within the recommendations provided by the Specialty Coffee Association of America (center point conditions) and the others with values that exceed or were lower than recommended: (9 bar/92 °C: center point; 7 bar/92 °C; 11 bar/92 °C; 9 bar/82 °C; and 9 bar/96 °C). Although all the coffees were prepared by an experienced barista, variations resulting from the manual preparation process were expected. To reduce this variability, we performed 8 extractions for each set of conditions and selected the 5 replicates for which the final weight of the extract was closest to 30 g, ending up with coffee weights in the range of 31.5 g ± 2 g.

2.2. Sampling setup

Volatiles were sampled using a previously used setup [22], with certain modifications (Fig. 1). The extracted coffee flowed into a custom built system that was heated to 96 °C to avoid condensation. Volatiles were drawn out using a vacuum pump and diluted 10-fold with dry compressed air to reduce their concentration to the dynamic range of the PTR-ToF-MS being used.

2.3. PTR-ToF-MS

A commercial PTR-ToF-MS 8000 instrument (Ionicon Analytik GmbH, Innsbruck, Austria) was used for all measurements. The diluted sample was introduced via a 90 °C heated sampling line into the drift tube operated at 2.3 mbar, 90 °C and 600 V drift tube voltage, resulting in an E/N value (electric field strength/gas number density) of 140 Townsend (Td, 1 Td = 10^{-17} cm^2/V s). PTR-ToF-MS data were recorded by TOFDAQ v.183 data acquisition software (Tofwerk AG, Thun, Switzerland). Mass spectra were recorded in the mass-to-charge (m/z) range of 0–300 with one mass-spectrum recorded every 2 s.

2.4. Data processing

Dead time correction, mass calibration, peak extraction and integration were performed using PTR-TOF DATA Analyzer software (v4.17) [23]. Duty cycle corrected signals were normalized to 10^6 H_3O^+ primary ions and the concentration in parts per billion by volume (ppbv) was estimated using 2×10^{-9} cm^3 s^{-1} as a reaction rate constant coefficient [24].

More than 500 mass peaks were detected in the range 0–300 m/z. Ions not related to the sample (O_2^+, NO^+ and water clusters) were eliminated, the background was subtracted and a concentration threshold of 1 ppb was set for further peak selection. This resulted in a reduction to 120 mass peaks that were present in all of the samples. From these peaks, 46 compounds (Table 1) were tentatively identified by comparing them to the literature [25,26].

2.5. Statistical analysis

The areas under the time–intensity curves were calculated for the 120 mass traces of each of the five replicates of the five different extraction conditions. Principal Component Analysis (PCA) was performed using mean centered and scaled areas. Analysis of Variance (ANOVA) was applied to assess the effect of the different extraction variables on the total area of the selected compounds using Tukey's Honest Significant Difference (HSD) post hoc test ($p < 0.01$). In order to identify compounds with similar dynamic behavior, first the time–intensity profiles of all the 120 m/z were normalized to their maximum intensity before performing self-organizing tree algorithm (SOTA). Subsequently the same SOTA analysis was performed on only the tentatively identified 46 VOCs. In addition the normalized time–intensity profiles of the 46 tentatively identified compounds were subjected to Hierarchical Cluster Analysis (HCA) using Ward's minimum variance method and half-squared Euclidean distances. All analyses were performed and all graphs were created using existing packages (clValid, multcomp, and ggplot2) and scripts developed in R [27].

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