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Time-resolved extraction of caffeine and trigonelline from finely-ground espresso coffee with varying particle sizes and tamping pressures

Michael Kuhn [a], Sandra Lang [a], Franziska Bezold [b], Mirjana Minceva [b], Heiko Briesen [a, *]

[a] TUM School of Life Sciences Weihenstephan, Chair of Process Systems Engineering, Technical University of Munich, Gregor-Mendel-Strasse 4, 85354, Freising, Germany

[b] TUM School of Life Sciences Weihenstephan, Chair of Biothermodynamics, Technical University of Munich, Gregor-Mendel-Strasse 4, 85354, Freising, Germany

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ABSTRACT

We investigated the extraction kinetics of caffeine and trigonelline from espresso coffee prepared in a commercial machine under realistic process conditions with varying particle sizes and tamping pressures of the coffee powder. On the one hand, it was found that the particle size significantly affects the extraction kinetics with smaller particles leading to a higher extracted amount of caffeine and trigonelline per collected coffee mass. Tamping pressure, on the other hand, has no detectable effect. Furthermore, the total extracted coffee mass was found to influence coffee composition as measured by the trigonelline/caffeine ratio. All data were sampled in triplicates with a high time resolution using a newly constructed sampling device. Finally, we introduced a new reduced model that describes the measured data well and contains only physically meaningful parameters. This work provides detailed data for better understanding the extraction of nonvolatile water-soluble components from espresso coffee, thereby aiding model development and validation. The presented simplified model may also prove useful for other related applications.

1. Introduction

Coffee is an important trading commodity (International Coffee Organization). Different beverages prepared from roasted coffee beans are widely consumed all over the world, and coffee consumption is still increasing (International Coffee Organization). Coffee produced from more than 9 million tons of raw beans was consumed in the year 2015. Among the different coffee beverages, espresso is one of the most popular. It is a highly concentrated drink obtained using a high water pressure of 8–11 bars applied during extraction and a short percolation time of 15–30 s for about 15–30 ml of espresso (Illy and Viani, 2005; Petracco, 2008); however, it must be mentioned that the values in the literature differ to some degree.

There has been much coffee research addressing the roasting process, sensory analysis, and physiological aspects of coffee consumption (Viani and Petracco, 2000; Illy and Viani, 2005; Eggers and Pietsch, 2008; Schilter et al., 2008). In contrast, this work focusses on coffee brewing alone, i.e. on percolation and the thereby achieved extraction of coffee components. Although many baristas have a lot of tacit knowledge about the effects of different extraction variables on the resulting coffee taste, reproducible quantitative data is still sparse, especially when it comes to time-resolved measurements. For the most part, the early studies investigating coffee extraction did not consider realistic process conditions. Instead, results were presented for batch conditions; i.e., coffee extraction was done in a stirred reactor. Under such conditions, the effect of particle size was examined and a significantly faster caffeine extraction for smaller particles was found (Spiro and Selwood, 1984), the extraction of caffeine under different degrees of roasting was studied (Spiro and Hunter, 1985), and the effect of intra-bean diffusion on caffeine extraction was evaluated (Spiro et al., 1989). Zanoni et al. (1992) observed different extraction phases while measuring concentrations of soluble substances, and Jaganyi and Madlala (2000) investigated the extraction kinetics of mineral ions and caffeine.

* Corresponding author.
E-mail address: briesen@wzw.tum.de (H. Briesen).

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An early work studying the effects of realistic coffee brewing conditions was reported by Bell et al. (1996). They found that both finer grains and greater amounts of coffee powder used lead to more cumulative caffeine in the cup. Hinz et al. (1997) presented data on the amount of total extracted solids over time for filter coffee and provided a simple mechanistic model for explaining this data.

In recent years, there have been renewed efforts to understand aspects directly related to the brewing process. Andueza et al. (2002) evaluated the effect of different extraction pressures on the quality of espresso coffee as reflected in physicochemical and sensory characteristics, whereas Mateus et al. (2007) investigated the wetting dynamics of coffee particles. Albanese et al. (2009) focused on the extraction temperature and found that extraction can be considered as an isothermal process with a true extraction temperature lower than the water reservoir temperature. Gloess et al. (2013) compared nine different extraction methods and found that the quality of coffee depends on the extraction method. Booth et al. (2012) show some evidence on the varying extraction kinetics of different coffee compounds; however, these data are not linked to the prevailing process conditions such as flow rate or particle size. Caprioli et al. (2014) quantified the extraction of caffeine, trigonelline, and nicotinic acid in espresso coffee under varying water temperature and pressure. They also did a preliminary investigation of the extraction kinetics at a low time resolution and found that after 25 s of extraction, further extraction merely dilutes the coffee.

Parenti et al. (2014) investigated the effect of different brewing techniques and found that capsule systems provide the best product reproducibility. Corrochano et al. (2015) studied the steady-state permeability of coffee beds and provided a corresponding modification of the Kozeny–Carman equation. Moroney et al. (2015) presented and validated a multiscale model for the extraction dynamics of filter coffee, but considered only the total solid content instead of single components. The same model is further analyzed in Moroney et al. (2016) and limiting solutions are derived. Moroney et al. (2016) also consider only the total solid content of coffee, even though the benefit of addressing the extraction of different coffee components is mentioned in the outlook. Sánchez-López et al. (2014, 2016) conducted an online analysis of the extraction of volatile organic compounds from espresso coffee by proton-transfer-reaction time-of-flight mass spectrometry. The first study found different extraction kinetics for different coffee compounds; the latter investigates the influence of temperature and pressure and found an increased extraction of volatile organic compounds for higher values of both variables.

This work focusses on caffeine and trigonelline. Both have been analyzed in many previous works as key components and important indicators of coffee quality. The extraction of caffeine has been addressed in several reports (Spiro and Selwood, 1984; Spiro and Hunter, 1985; Spiro et al., 1989; Zanoni et al., 1992; Bell et al., 1996; Jaganyi and Madlala, 2000; Albanese et al., 2009; Gloess et al., 2013; Caprioli et al., 2014; Parenti et al., 2014); trigonelline has been also investigated previously (Farah et al., 2006; Caprioli et al., 2014; Parenti et al., 2014).

Trigonelline and caffeine are among the components with the highest mass fraction in coffee (Viani and Petracco, 2000; Illy and Viani, 2005). Both are nonvolatile, water soluble, and bioactive (Buffo and Cardelli-Freire, 2004; Caprioli et al., 2014). Typical values of caffeine content in dried green Arabica and Robusta coffee beans are 1.2 and 2.4 wt%, respectively. Trigonelline is present at about 1.0 wt% in green Arabica and 0.7 wt% in green Robusta beans. Caffeine content is unaffected by roasting whereas trigonelline decomposes to other substances and is thereby reduced by 30–80% in mass depending on the degree of roasting. Typical values in a coffee cup extracted from 7.5 g of roasted ground coffee at an extraction yield of 22% lie in the range of 50–150 mg caffeine and 30–60 mg trigonelline (Caprioli et al., 2014).

As can be seen from the literature review, there is a gap in current knowledge with respect to the detailed extraction kinetics of nonvolatile espresso components under realistic process conditions.

We, therefore, study in this paper the extraction of caffeine and trigonelline from espresso coffee brewed in a commercial machine. Our aim is to provide reproducible data sampled with a high time resolution. Furthermore, a simplified model, containing only physically meaningful parameters, is derived and applied. The model aids a mechanistic understanding of coffee extraction and paves the path for more complex modeling approaches.

2. Materials and methods

2.1. Chemicals

Caffeine (analytical standard) and trigonelline (analytical standard), both with a purity >99%, were obtained from Sigma Aldrich (Taufkirchen, Germany). Methanol for HPLC analysis (HiPerSolv CHROMANORM) was purchased from VWR Chemicals (Ismaning, Germany).

2.2. Milling and sieving

Coffee (Espresso Nicaragua, 100% Arabica, variety Caturra) was obtained in 250 g packages from a local roaster (Caffé Fausto, Munich, Germany). All beans were freshly roasted with the same temperature profile, and the sealed packages were stored for no longer than four weeks before the experiments. Packages once opened were not stored again to guarantee fresh ground coffee quality for every set of experiments. A precision balance (FB6CCE-H, Sartorius AG, Göttingen, Germany) was used to weigh 14 g of freshly milled beans for each experiment that was conducted; this is appropriate as the typical amount of ground coffee beans for a double espresso lies in the range of 10–16 g (Illy and Viani, 2005). Milling was done with a professional espresso coffee mill (Combo Coffee Grinder and Grater FMC6, Fama Industrie, Rimini, Italy) for which the reproducibility of the milling results was assured by preliminary experiments. Particles sizes were chosen in order to achieve manageable flow rates during coffee extraction under the process conditions described subsequently. For this reason, a comparatively fine ground was used. For some experiments, particles were sieved (vibrational sieving tower AS 200, Retsch, Haan, Germany) to achieve narrower particle size distributions. Sieves with mesh sizes of 250, 280, 315, and 355 μm were used, as also reflected in the values shown in Table 1. A sieving time of 25 min and sieving intervals of 10 s with an amplitude of 1.2 mm were used. The ground coffee was sieved together with sieving aids (three rubber balls with a diameter of 20 mm) to reduce agglomeration of coffee particles. Mass conservation on all sieves was assured and a brush was used to clean sieves of adhering particles which were also added to the corresponding sieve fractions. In preliminary experiments, the sieving strategy was validated by repeated sieving runs and subsequent particle size analyses, assuring stable results. All particle sizes were measured by laser diffraction under dry-dispersed conditions (HELOS, Sympatec GmbH, Clausthal-Zellerfeld, Germany). For one basic experimental scenario, particle shapes were quantified by quasi-static image analysis (QICPIC, Sympatec GmbH, Clausthal-Zellerfeld, Germany).