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Mark Al-Shemmeri
Email: mxa118@student.bham.ac.uk
School of Chemical Engineering
University of Birmingham
Birmingham B15 2TT, UK

Kit Windows-Yule
Email: c.r.windows-yule@bham.ac.uk
School of Chemical Engineering
University of Birmingham
Birmingham B15 2TT, UK

Estefania Lopez-Quiroga
Email: e.lopez-quiroga@bham.ac.uk
School of Chemical Engineering
University of Birmingham
Birmingham B15 2TT, UK

Peter J. Fryer*
*Corresponding author
Email: p.j.fryer@bham.ac.uk
School of Chemical Engineering
University of Birmingham
Birmingham B15 2TT, UK

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Mark Al-Shemmeri[1,2], Kit Windows-Yule[1], Estefania Lopez-Quiroga[1], Peter J. Fryer[1*]

[1] School of Chemical Engineering, University of Birmingham, B15 2TT, UK.

[2] Jacobs Douwe Egberts, R&D Offices, OX16 2QU, UK.

Abstract

Coffee roasting is a heat treatment process that transforms green coffee into a product that can subsequently be ground and brewed. Understanding roasting is critical in developing new downstream processes and formulations, as well as in optimising existing ones. Positron Emission Particle Tracking (PEPT) allows tracking of particles in process equipment and has been used here to characterise particle dynamics of coffee beans within a spouted bed roaster subject to varying air-to-bean ratios without roasting. Occupancy profiles associated with each air-to-bean ratio have been determined and two distinct regions identified: (i) a *dense* bean bed of high occupancy (ii) a *dilute* freeboard of lower occupancy. Results also revealed the effect of coffee density on particle dynamics within the roaster. Overall, this work demonstrates that PEPT can be a useful tool to generate data regarding granular flow patterns in roasters that might be used to improve existing heat and mass transfer models for roasting.

Keywords: Positron Emission Particle Tracking (PEPT); spouted bed of coffee beans; particle motion modelling; air-to-bean ratio; coffee roasting degree and density

1 Introduction

Coffee roasting is a heat treatment process that transforms green coffee via changes in hydration, chemical composition and microstructure. During roasting, coffee is subject to high temperature air flows, applied via specific time-temperature roasting profiles, so moisture content decreases in an endothermic drying process (Alessandrini et al., 2008; Pittia et al., 2011; Romani et al., 2012; Schenker, 2000). These time-temperature profiles are designed based on empirical evidence, trial and error, or simply the experience of the roast master. Manipulations of temperature, air flow, batch size and roast time all influence the roasting profile; the ability to manipulate these parameters allows the coffee's characteristic flavour and aroma to be developed (Hoos, 2015; Rao, 2020) – complexity of profile manipulation has been discussed in detail by Hoos (2015); Rao (2014, 2020).

Once the free moisture has been removed in the early stages of roasting the colour of the coffee gradually changes from pale green to yellow (Geiger et al., 2005; Rao, 2014; Schenker, 2000; Wang and Lim, 2012). As the coffee temperature increases beyond 170^{o}C-190^{o}C, the initially endothermic roasting process becomes exothermic, with the beginning of Maillard reactions, causing the colour to shift from yellow to brown (Schenker, 2000). The combined effect of heat generation in the bean's core – leading to water vapour within the bean – and the formation of CO_2, increases the internal pressure until the bean's structure fails, releasing an audible "crack" that coincides with a significant expansion in both volume and surface area (Geiger et al., 2005; Rao, 2014; Schenker, 2000; Wilson, 2014). The period after this *'first crack'*, described in specialty coffee as the *development time*, has been highlighted as being critical to control due to rapid changes in physicochemical properties (Hoos, 2015). Beyond first crack, oils migrate to the coffee's surface and carbon dioxide accumulates until *second crack* occurs (Rao, 2014; Wilson, 2014; Yergenson and Aston, 2020).

Once the desired end-point of the roast has been reached the coffee is cooled by either cool air or quench water (Baggenstoss et al., 2008; Schenker, 2000).

The physicochemical transformations that occur during roasting are numerous and inter-related. Monitoring changes in physical and chemical properties of coffee during roasting is critical as rapid transformations in colour, volume and density occur through both first crack and *development time* (Alessandrini et al., 2008; Bustos-Vanegas et al., 2018; Garcia, et al., 2018; Yergenson and Aston, 2020). The commercial need is to understand and predict how to control the roast to improve product quality and process efficiency. This can be achieved either using empirical correlations, or through physics-based predictive models.

Particle and fluid interactions govern heat and mass transfer (Bergman et al., 2011), yet little work has been done to characterise coffee roasting. Whilst both air flow and batch size are critical to coffee development and roasting (Kwak et al., 2017), there is little literature on their effect on coffee during roasting aside from those documented by Rao (2014, 2020). Cristo et al. (2006) and Resende et al. (2017) used photography in transparent drums to visualise dynamic behaviour of coffee in rotating drums.

Computational Fluid Dynamics (CFD) can be used to model and predict flow behaviour in *dilute* granular systems (Abdul Ghani et al., 2019; Alonso-Torres et al., 2013; Chiang et al., 2017; Oliveros et al., 2017). Coupled CFD and Discrete Element Method (DEM) can simulate lumped and distributed temperature distributions within spouted bed roasters (Azmir et al., 2020; Bruchmüller et al., 2010) but is often difficult to validate. Bruchmüller et al. (2010) established a DEM model to describe the development of temperature and moisture within a fluidised bed of spherical particles during roasting. This enabled single-bean resolution of temperature and moisture distributions within the batch, founded on fundamental physical phenomena. Azmir et al. (2020) studied a similar system at lower temperatures (50-200°C) incorporating particle shrinkage – effects of initial moisture content, density and particle size were highlighted.

PEPT is a non-invasive technique that can characterise flow behaviour within granular systems. The trajectories of particles labelled with positron-emitting radioisotopes can be tracked in three-dimensions with high temporal and spatial resolution (Windows-Yule et al., 2020). The principles of PEPT are described in detail by Parker et al. (1993) and Parker (2017), while PEPT's best practices and applications were recently reviewed by Windows-Yule et al. (2020). PEPT measurements are typically performed on steady-state systems in real process equipment (Windows-Yule et al. 2020) and thus experimental design includes part-processed products to emulate the changes in material properties that occur during operation. Characterisation of particle dynamics could give the ability to fundamentally describe heat and mass transfer independent of roaster design. For industry, the need is to transform development and innovation of both roasting process and product into an off-line exercise.

Here, PEPT has been used to study the particle dynamics of coffee in a pilot-scale spouted bed roaster that is representative of full-scale systems, with the aims of (i) understanding the granular flow patterns in the roaster and (ii) showing that the resulting data provides boundary conditions that might be integrated within a suitable thermal model to predict time-temperature profiles during roasting. The experimental design was selected to emulate changes during roasting. As PEPT measurements require long data capture times, and high temperature roasting incurs rapid transformation of the coffee's physicochemical properties, PEPT measurements of real roasting are not possible. By studying coffees of different roast degrees and densities (thus emulating the changes in physicochemical properties during roasting), the corresponding particle dynamics at different stages of real roasting can be inferred.

2 Materials & Methods

2.1 Coffee beans

Before PEPT measurements, batches of 350g of Kenyan Arabica coffee were isothermally roasted in a spouted bed roaster (RFB-S, Neuhaus Neotec) at a temperature of 250°C and a fan frequency of 48 Hz (i.e., inlet air velocity of 7.2 m s^{-1}). Part-roasted and roasted samples were obtained by roasting for 2 mins 18 s (138 s) and 4 mins 38 s (278 s), respectively; green coffee samples were not roasted. Coffee samples from triplicate roasts were combined and well mixed prior to PEPT studies to minimise variations between batches.

Intrinsic density was determined by measuring the coffee bean's principal dimensions (digital calipers, IP54, Perciva) and mass (XSR204, Mettler-Toledo); 25 beans from each sample set were measured. From the bean dimensions, a (width), b (depth) & c (length) (mm), bean volume, V_b (mm^3) was calculated assuming bean geometry is that of a hemi-ellipsoid ($V_b \approx \frac{\pi abc}{6}$). Bulk density was calculated from the measured mass (Lunar balance, Acaia) of coffee that occupies a 250 ml beaker, where beans settled freely. The top of the beaker was smoothed to ensure a level fill and measurements were repeated in triplicate using aliquots of each sample set. Coffee properties are presented in Table 1.

2.2 Coffee roaster

The same spouted bed roaster that produced the roasted coffee samples was used here for flow studies. A simplified schematic of the roasting chamber is presented in Figure 1 (a). To support the description of the system volume, Figure 1 (b) highlights the orientation of the roaster within the space between gamma-ray detector heads. The centre of the roasting chamber was used as the origin for the data.

Both the velocity and mass flow rate of air inputs to the roaster were determined as a function of the fan frequency using a hot-wire anemometer (405i, Testo) installed on the inlet air pipe (ø 60 mm) between the blower and heating element. The roaster was operated at ambient temperature (c. 25°C) with fan frequencies of 30-60 Hz at 5 Hz intervals for 10 mins. An average velocity for each fan frequency was calculated and used to determine inlet air mass flow rates. Table 2 outlines the corresponding air velocities and mass flow rates for several fan frequency set points.

2.2.1 Roaster fill volume

The volume occupied by a static bean bed (i.e., coffee beans within the roasting chamber with no applied heat, or airflow) was determined using the coffee's bulk density, specified batch size and roaster geometry. The bean bed was assumed uniform along the *z direction*, according to Figure 1 (b), with a depth of 9.8 cm. The equivalent area occupied by a static bed of beans in the plane *xy* of the roaster, according to Figure 1 (b), is thus a function of the coffee's batch size and bulk density, in addition to the geometry and depth of the roaster. Table 3 outlines the static bean bed area according to batch size and coffee density.

2.3 Positron Emission Particle Tracking (PEPT)

2.3.1 Experimental setup & tracer labelling

The spouted bed roaster was placed between two detector heads of a modified ADAC Forte positron camera, such that the roasting chamber falls at the centre of the camera's most sensitive region, parallel to the detector heads - ensuring both a maximal acquisition rate and precision. Further details of the positron camera are given in Parker et al. (2002) and Windows-Yule et al., (2020).

A single coffee bean was selected from each sample set; principal dimensions of the selected particles were checked to be within one standard deviation of the batch's mean. Selected particles were indirectly labelled by pipetting 2 ml of water – containing ions of Fluorine-18, a β^+-emitting radioisotope - onto the particle's surface (Parker, 2017). After allowing 15 mins for absorption of irradiated water, excess water, determined gravimetrically, was removed by drying the coffee bean under a heat lamp. A balance with 0.1 mg precision (XSR204, Mettler-Toledo) was used to measure the mass before and after labelling, ensuring that the two agreed to within the stated precision of the balance. The labelled coffee bean was returned to the sample set and placed in the roaster.

All experiments were conducted in accordance with the Positron Imaging Centre's Local Rules, under the supervision of a trained radiation protection supervisor.

2.3.2 Experimental procedure

The experimental design intends to emulate roasting through the study of coffee beans of different roast degrees and densities and reflects realistic variations of air-to-bean ratio that a roaster might employ. Air-to-bean ratio is defined as the ratio of the total mass of air input to the roaster during a roast (i.e., the product of the mean air mass flow rate and total roast time) to the mass of the batch. The experimental conditions considered a range of batch sizes (200, 350 and 500 g), air flows (fan frequencies of 30, 39, 48 and 65 Hz) and roast degrees (green, part-roasted and roasted). Minimum airflow for spouting of 350 and 500 g batches of green coffee corresponded to fan frequencies of 39 and 48 Hz, respectively. As spouting is required for roasting conditions to be safely employed in a commercial setting, only fan frequencies of 48 and 65 Hz were studied for 500g batch sizes; fan frequencies of 39, 48 and 65 Hz were studied for 350g batches and 30, 48 and 65 Hz for 200g batches.

For the system to be considered ergodic, data was captured over a period sufficient for the tracer particle to fully explore the roasting chamber. Thus, once particle motion was established at ambient temperatures (c. 25^{o}C), data was captured for 60 mins.

2.3.3 Time average analysis of cartesian co-ordinates

For steady-state systems, it is assumed that the time averaged behaviour exhibited by a single particle in a homogenous system is representative of the ensemble-averaged behaviour of all particles in the system (Wildman et al., 2000). From this, the system can be considered ergodic and therefore it is expected that the fractional residence time of the tracer in any given region, is directly proportional to the typical fraction of total particles in that region at any given point in time (Windows-Yule et al., 2020).

Experimental datasets – containing Cartesian coordinates at time intervals of 0.01-0.1 milliseconds (dependent on tracer activity) – were segmented to account for systemic variability such that each 60 min experiment generated three 20 mins datasets. These time-segmented datasets were subsequently analysed in MATLAB (2020a, MathWorks). For analysis of ergodic systems, with the allowance of sufficient time for data capture and appropriate sizing of mesh element dimensions, the decay of the tracer's activity, with a half-life of 109 mins, is assumed to have no significant impact on the resultant time-segmented occupancy profiles.

2.3.4 Occupancy profiles

Occupancy of the system is determined by division of the system's volume into uniform elements (pixels in 2D, voxels in 3D). Here, a system of 100x100 elements in 2D was established as depicted in Figure 2 (a), where mesh element dimensions were approx. equivalent to the camera's intrinsic spatial resolution. For a tracer moving at 7 m s^{-1} (equal to the mean inlet air velocity of the roaster) the tracer can be located within approx. 3.5mm (Parker et al., 2002), so mesh element dimensions of 3.5x3.5 mm in 2D were used. Occupancy profiles shown in Figure 2 (b) – where high occupancy regions are red; low occupancy regions are dark blue – are expressed as a fraction of total experimental time and are determined knowing the residence time of the tracer in each element; the occupancy within each element is proportional to the mean packing density of particles (Windows-Yule et al., 2020).

2.3.5 Delineation and resolution of occupancy profiles

The occupancy profiles in Figure 2 (b) reveal the existence of two different regions: a *dilute* (i.e., low occupancy) freeboard and a *dense* (i.e., high occupancy) bean bed. The sum of these two regions is defined here as the area of the roaster in a given two-dimensional plane (A_o) that is occupied under the specified roasting conditions, and it is determined from the number of non-zero elements in a given two-dimensional plane (n_{nze}) and the elemental area (A_e) of occupancy profiles (Figure 2 (b)) as follows:

$$A_o = \sum n_{nze} A_e \quad \text{Eq. (1)}$$

The bean bed area is determined via application of an Otsu method (Otsu, 1979) to normalised probability distributions of one-dimensional (in *y*) occupancy profiles – implemented in MATLAB (2020a, MathWorks). Threshold values were determined for each occupancy profile - as illustrated in Figure 3 - as the value is dependent on the distribution of fractional residence times observed for each occupancy profile. It is assumed that occupancies below the threshold value are associated with the *dilute* freeboard, while occupancies over that threshold value relate to the *dense* bean bed. The area occupied by the bean bed (A_b) is calculated using a similar approach to that used to calculate the overall occupied area (i.e., Eq. (1)).

2.3.6 Particle trajectories, residence times and spatial velocity distributions

Spatial velocity distributions are used here to identify granular flow patterns in the *dilute* freeboard and *dense* bean bed. Both the velocity and time spent by a particle in each region (i.e., residence time), can be determined using the individual particle trajectories – Figure 2 (c) shows consecutive particle trajectories defined using the bed's location. Beans crossing the bean bed-spout interface twice in rapid succession caused a large number of low residence times, so individual particle trajectories corresponding to residence times below 0.01% of maximum residence time in each region for a specified condition were omitted. Particle velocities were then determined as described by Windows-Yule et al. (2020).

3 Results

During roasting, bean properties vary significantly. To study these changes and the effects they have on coffee bean particle motion, experiments were conducted at ambient temperatures where the roaster was filled with green, part-roasted and fully-roasted beans (prepared prior to PEPT measurements as discussed above). The data sets thus show the changes in behaviour that will occur during roasting.

3.1 Occupancy and velocity profiles in the roaster

Both occupancy and velocity profiles have been obtained from PEPT data as explained in Section 2 for different bean densities (i.e., green, part-roasted and roasted), air flow frequencies (i.e., velocities) and batch sizes, and are presented next. Overall, these results define two different occupancy regions (i) a *bed* of high solids fractions through which beans move slowly (<0.5 m s-1) together with (ii) a spout of beans – the *freeboard* – moving rapidly (0.5-1.5 m s-1) upwards at the air inlet which then fall to the surface of the bed.

3.1.1 Effect of bean density

Figure 4 shows PEPT data for 350g batches of green, part-roasted and roasted coffee at a constant fan frequency of 48 Hz, thus indicating how particle (i.e., bean) motion in the roaster changes as a function of bean density – during a real roast, the density of the beans would change reflecting that of the studied green, part-roasted and roasted beans. Occupancy plots, i.e., Figure 4 (a)-(c), show low occupancy values for the upper part of the roaster (the freeboard), while occupancy at the bottom of the chamber decreases with bean density. For example, green beans, with higher bean density, tend to occupy the bottom region of the roaster, forming a small bed of high occupancy (red region in Figure 4 (a)). Fully roasted beans, with lower bean density, form larger beds, but less densely occupied (green region in Figure 4 (c)) – lower density makes beans easier to fluidise and spout.

Velocity profiles presented in Figure 4 (d)-(f) reveal that there is a general rotation of the beans around a point within the bed near the spout region (most evident in Figure 4 (c)), with the highest bean velocities corresponding to the rise and fall of beans in the spouted bed freeboard.

3.1.2 Effect of air flow

Figure 5 shows PEPT data for 200g batches of green coffee at different fan frequencies, thus showing how bean motion changes with airflow. As air flow increases, the total area occupied by coffee in the roaster significantly increases (see Figure 5 (a)-(c)), as higher air flows ease fluidisation. The corresponding velocity profiles (see Figure 5 (d)-(f)) also show an increase of bean velocity in the freeboard with increasing airflow; the high occupancy region (i.e., the bed) is again slow moving. Figure 5 (f) shows the rotational nature of the flow most clearly. At this highest airflow, a new, circulating flow regime with no true bean bed was established (Figure 5 (c)). This shows in the reduced red region of high occupancy (see Figure 5 (c)) and the corresponding velocity profile (see Figure 5 (f)), which shows the rotation of beans around a point closer to the spout. This phenomenon is unique to these conditions due to the combination of a high coffee density and high air-to-bean ratio - smallest batch and highest fan frequency.

3.1.3 Effect of batch size

Figure 6 shows PEPT data for 200, 350 and 500g batches of roasted coffee at a fan frequency of 48 Hz, thus showing how beans motion changes with batch size. For these conditions, the region with the higher occupancy levels – red area at the bottom of the roaster in Figure 6 (a) - becomes larger and less dense as batch size increase - see Figure 6 (b)-(c). Bean velocities associated to these bed regions are the slowest within each of the systems, as shown in Figure 6 (d)-(f).

For larger batches of roasted coffee (see Figure 6 (c)), two occupancy bands are visible in the bean bed. The larger band in the centre of the bean bed (see Figure 7 (b)), corresponds to beans that follow the modal freeboard trajectory, from the spout into the bed - shown by the densely populated particle trajectories in the top part of the roasting chamber (visible in Figure 7(a)) - and fall downward to the spout, parallel to the wall. The smaller band is formed at the top of the bean bed, near the spout, and is caused by beans that are propelled with less force, leading to scattered motion in this region, as shown in Figure 7 (b).

3.1.4 Combined effect of coffee density, air flow and batch size on roaster occupancy

Figure 8 (a)-(c) plots the variation of total occupied area of the roasting chamber for all experimental conditions obtained from PEPT data - note that bulk density decreases with a higher roasting degree (see Table 1). The occupied area of all batch sizes tends toward the capacity of the roasting chamber as airflow increases. For low air-to-bean ratios (i.e., large batch size and low airflow), the maximum area is achieved at lower airflow (Figure 8 (a)-(c)) due to the greater fill volumes (i.e., larger occupied areas in plane *xy*) for larger batch sizes. Occupied area at high airflow (65 Hz) decreases with batch size and increases as coffee density decreases. For moderate airflow (48 Hz), occupied area increases as coffee density decreases, yet occupied areas of part-roasted and roasted coffee systems are not significantly different, thus the impact of batch size is not significant for part-roasted and roasted coffee.

Figure 8 (d)-(f) plots the variation in bed area for all experimental conditions. Lower density coffees (i.e., roasted beans that have lost mass, but increased in size) are more easily spouted than the higher density (green) coffee, and thus bean bed mass decreases with density, however bed area increases with decreasing density due to volumetric expansion (see Table 2). For all conditions, bed area increases with batch size; for a given batch size, while increasing airflow decreases the bed area, the effect is less significant than the change in density.

3.1.5 Residence time

Figure 9 presents cumulative distributions of residence time that result from changes in coffee density, airflow and batch size. The data is presented as the residence times in the bean bed, the freeboard, and recirculation times (from spout-to-spout); residence times in the bean bed and freeboard were identified as shown in Figure 7.

Figure 9 (a) shows that as coffee density decreases, residence times in the bed increase, while freeboard residence times decrease slightly. As coffee bean density decreases, beans are more easily fluidised, and have faster freeboard velocities leading to smaller residence times (Figure 9 (b); also seen in Figures (4)-(6)).

Figure 9(d-f) shows bean bed residence times increase at lower airflows; they also indicate that, for roasted coffee, the variation in residence time (as seen in Figure 7 (a)) decreases with airflow. Spout-to-spout recirculation times presented in Figure 9 (b) are mostly affected by bean bed travel as particle velocities in the freeboard are much greater than in the bed for all bean densities.

Under moderate airflow (48 Hz), Figure 9 (g) reveals that the larger the batch size, the greater the bean bed residence time: greater fill volumes (i.e., larger bed areas in plane *xy*, as shown in Figure 6) result in longer bean bed travel distances from the surface to the spout. For moderate airflows (48 Hz), batch sizes of 500 and 200g roasted coffee correspond to bed heights of 17.5 and 11.9 cm, respectively. As bed height increases with fill volume, the downward freeboard travel distance decreases, thus in the freeboard, larger batch sizes are associated with shorter residence times.

3.2 Bean dispersion

The occupied area of coffee in the roasting chamber is defined by the dispersion of the beans propelled from the spout, i.e., the variation between individual freeboard trajectories, such as those shown in Figure 7 (a) (Windows-Yule et al., 2020). The distribution of the vertical component for coffees of different densities in a 200g batch at moderate airflow (48 Hz), is presented in Figure 10 (a), and that for the horizontal component is shown in Figure 10 (b). It can be seen that (i) for green coffee, there is very little vertical distance travelled, reflecting the low fluidisation of high-density particles, whilst there is much greater vertical displacement of the roasted, and thus lighter, coffees, (ii) the horizontal distance travelled by beans increases as the coffee density decreases.

4 Implications for Heat Transfer

4.1 Regional variation of heat transfer

Bean bed and freeboard heat transfer behaviour will be different due to the different flow patterns in each region that have been revealed in this work:

(i) Freeboard region. The heat transfer coefficient in the spout will be high as the beans will be subject to significant air-to-bean convective heat transfer. The coffee temperature will also increase rapidly through contact with the hottest air.

(ii) Bean bed region. Within the bed, heat transfer is governed by a number of mechanisms, including: bean internal conduction, bean-to-bean surface conduction (contact), bean-to-bean surface radiation (non-contact), air-to-bean convection, convection in voids, and the effective thermal conductivity of the bed (Díaz-Heras et al., 2020).

These two regions will present very different heat transfer mechanisms and depending on the intended product, both present positive and negative impacts on potential cup quality. A thermal model for roasting will combine the particle motion data's residence times in both regions with thermal boundary conditions appropriate to each; beans that flow from spout-to-spout - through the roaster - will experience a range of conditions.

As the temperature difference between bean and air decreases, so will heat transfer (Brown and Lattimer, 2013). In the bed, the region adjacent to the spout will likely be at a higher temperature than the centre of the bed. The temperature of the metal will be close to that of the adjacent beans.

The increase in total occupied area during roasting, and thus increased fraction of beans in the freeboard, indicates that a greater fraction of beans will be subject to convective heat transfer in the latter stages of roasting. Cheng et al. (2020) found that heat conduction through bed voids increases with bed porosity and is significant for systems where the air to particle conductivity ratio is less than 5, as it is here. Therefore, as bed fluidisation and porosity increases, conductive heat transfer through the voids can be expected to increase, improving bed heat transfer.

4.2 Heat transfer efficiency

Although increasing heat transfer rates is desirable to improve productivity (due to shorter process times) and yield (as a faster roast typically has a lower mass loss), the impact on flavour is a concern - faster roasts tend to provide underdeveloped coffees. For commercial roasting it may be best to start with moderate air flow, and to reduce it as coffee density changes to maintain a consistent occupancy profile. Reduction of air flow during roasting also acts to supress exothermic reactions that are initiated around first crack (Schwartzberg 2002) – seen in a sudden increase in the time-temperature roasting profile. This will reduce both batch inhomogeneity, and potentially energy consumption, provided the necessary changes to maintain similar time-temperature profiles are minimal.

To increase bean-to-bean conductive heat transfer rates (similar to those in drum roasters), process conditions that employ a large bean bed area with little bed fluidisation are needed; to improve air-to-bean convective heat transfer, as well as convection through bean bed voids, air flow should be maximised to maintain a large fraction of beans in the freeboard – this method is recommended to improve batch consistency.

4.3 Impact on temperature measurement

The complexity of the flow pattern will affect the measured temperature, depending on where that temperature was measured. Thermocouples in the bean bed will measure a combination of bean and air temperature. At the start of roasting the temperature of the air in the roasting chamber will be higher than in the beans but, as the roast progresses, bean temperature will approach that of the air. As the packing density around the thermocouple will be affected by the local flow behaviour, heat transfer from the bean bed environment to the thermocouple will be affected. It is expected that as the packing density decreases during roasting (i.e., the bed expands and becomes more fluidised) there would be increased contact area between the thermocouple and the air, and a decreased contact area between the thermocouple and beans. The measured 'bean' temperature will thus be overestimated, as the air temperature is greater than the beans. This problem adds complexity to comparing time-temperature profiles for dissimilar roasting conditions.

4.4 Comparison with previous studies

There are some models for roaster behaviour. Single-bean CFD simulations (Chiang et al., 2017) – considering convective heat transfer only – suggested that the uniformity of in-bean temperature distributions increases during the first 1 min 10 s (100 s) of roasting. The impact of bean volume on the temperature and moisture distributions (Abdul Ghani et al., 2019) endorsed adjustment of time-temperature roasting profiles according to the size of green coffee beans. In each of these studies, changes in bean volume during roasting were not considered. The PEPT measurements – particularly those in Figure 8 – suggest that changes to airflow should be performed according to the volumetric expansion of coffee during roasting. Such changes are expected to promote the uniform development of moisture and colour within the bean – although lower energy input increases process time.

For heat and mass transfer simulations, Bustos-Vanegas (2015) implemented subroutines to describe (i) density changes as a function of moisture (ii) volumetric expansion as a function of both moisture and applied air temperature during roasting. Although the estimated global heat transfer coefficients were discussed and validated (Bustos-Vanegas 2015), PEPT measurements

– particularly those in Figure 8 – suggest that for a system with constant airflow, as bean density decreases a greater number will be propelled into the *dilute* freeboard, where convective heat transfer is dominant – the global heat transfer coefficient would increase as roasting proceeds.

CFD-DEM studies of grain drying (Azmir et al., 2020) observed convection-dominant drying at high air velocities in a fluidised bed, with conductive heat transfer increasing as airflow decreases. DEM simulations of coffee roasting in fluidised beds (Bruchmüller et al., 2010) suggest that the global heat transfer coefficient is greatest during the intermittent lifting of beans into the freeboard, resulting in periodic variation of the heat transfer coefficient during roasting. The PEPT measurements shown here also suggest differences in heat transfer in the spouted bed roaster. Differences in the rate of convective heat transfer in the bed and freeboard will create periodic variations of the single-bean heat transfer coefficient due to cyclic particle motion. The next stages of work will be to develop a roasting model using the PEPT data as a basis.

5 Conclusions

PEPT has been used to capture particle dynamics of coffee beans inside a spouted bed roaster at ambient temperatures. Coffees of different roast degrees and densities were studied to emulate the effects of roasting, while the batch size and air mass flow rate were varied to study the impact of air-to-bean ratio on particle dynamics.

PEPT data was used to identify the location and subsequent trajectories of a single bean with time. Through calculation of fractional residence times, occupancy of the roasting chamber revealed two different regions: a *dense* bean bed and a *dilute* freeboard. The effect of changing air flow, batch size and bean density has been demonstrated. Beans become less dense and the flow pattern changes as roasting proceeds, which changes the heat transfer characteristic of the roaster in both regions (i.e., bean bed and freeboard).

The potential to optimise heat transfer during roasting (i.e., increase efficiency) has been discussed. Overall, this work demonstrates that PEPT can be a useful tool to understand granular flow patterns in roasters. The identified evolution of regional mass fractions and corresponding residence times provide quality data (i.e., dynamic boundary conditions) to be used to improve heat and mass transfer models for roasting.

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Author statement

Mark Al-Shemmeri: Investigation, Experimental work and analysis, Writing – original draft; Kit Windows-Yule: Experimental work and analysis, Writing – review & editing; Estefania Lopez-Quiroga: Formal analysis, Supervision, Writing – review & editing; Peter Fryer: Conceptualization, Writing – review & editing, Supervision, Funding acquisition.

Declaration of competing interests

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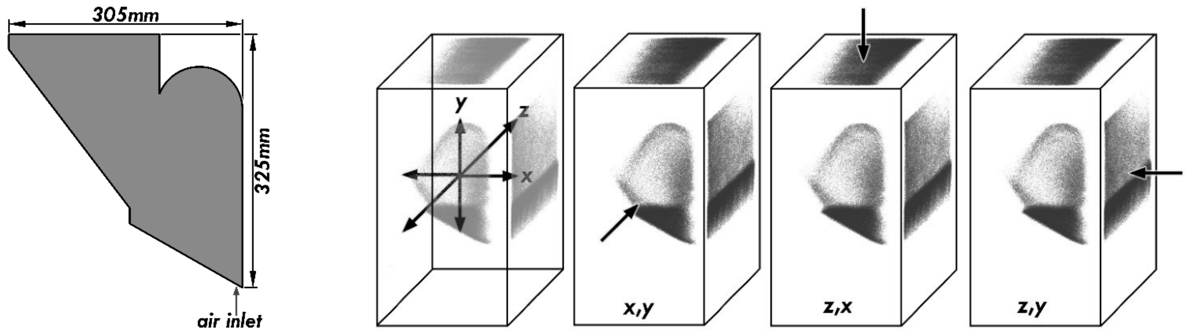
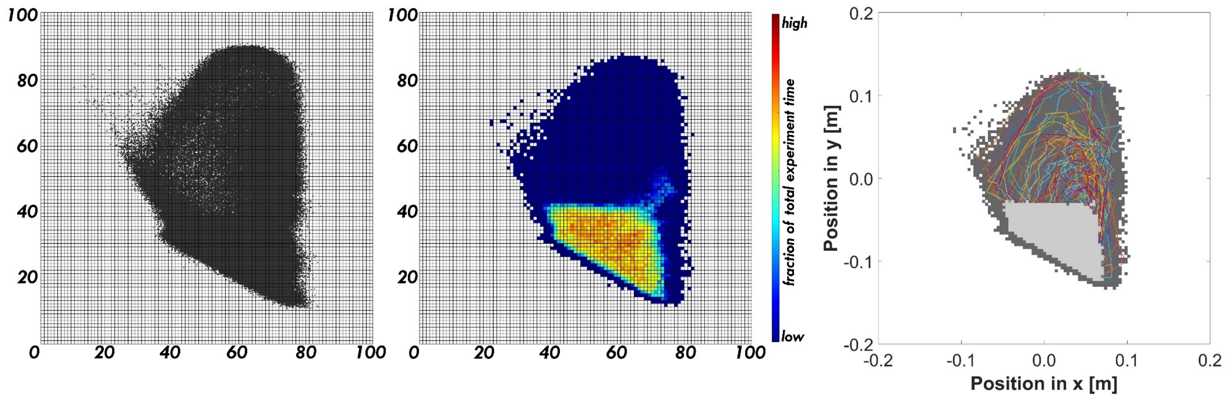
FIGURES



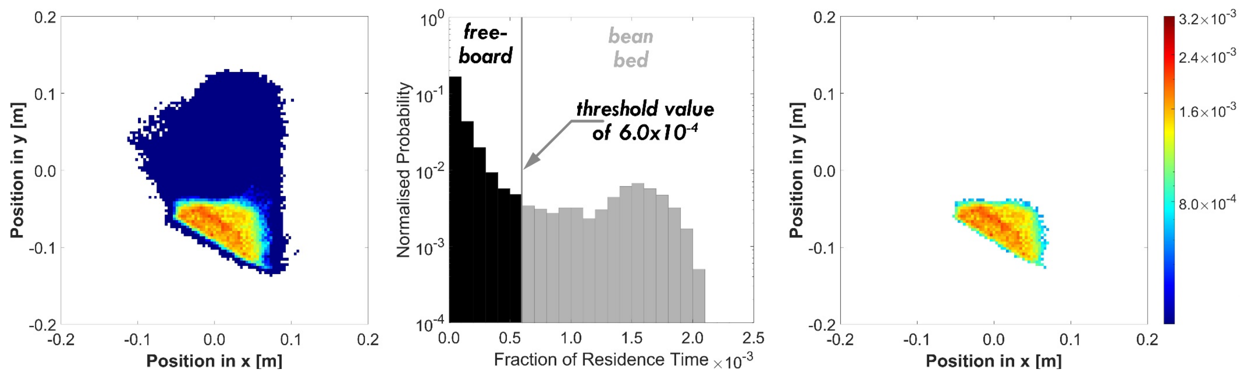
(a) (b)

Figure 1. Description of roasting system, outlining (a) a simplified schematic of the spouted bed roasting chamber and (b) established orientation of system volume using a simplified, cubic schematic of the roaster overlaid with recorded tracer positions from a single run (200g of part-roasted coffee beans at a fan frequency of 48 Hz).



(a) (b) (c)

Figure 2. Subdivided system volume of 100x100 elements of 3.5x3.5 mm - in plane *xy* - overlaid with (a) all experimental data points and (b) the occupancy profile of an individual run, from which (c) an example of individual particle trajectories (multi-colour) - tracked from the spout, through the freeboard (dark grey) until their return to the bean bed (light grey) - can be identified. Data displayed in (b) and (c) relates to a 200g batch of part-roasted coffee beans where the roaster fan frequency was set to 48Hz.



a b c

Figure 3. Visualisation of the Otsu method thresholding process to delineate a) total occupancy via determination of a threshold value based on b) normalised probability distributions of fractional residence time in *y* to reveal c) bed occupancy.

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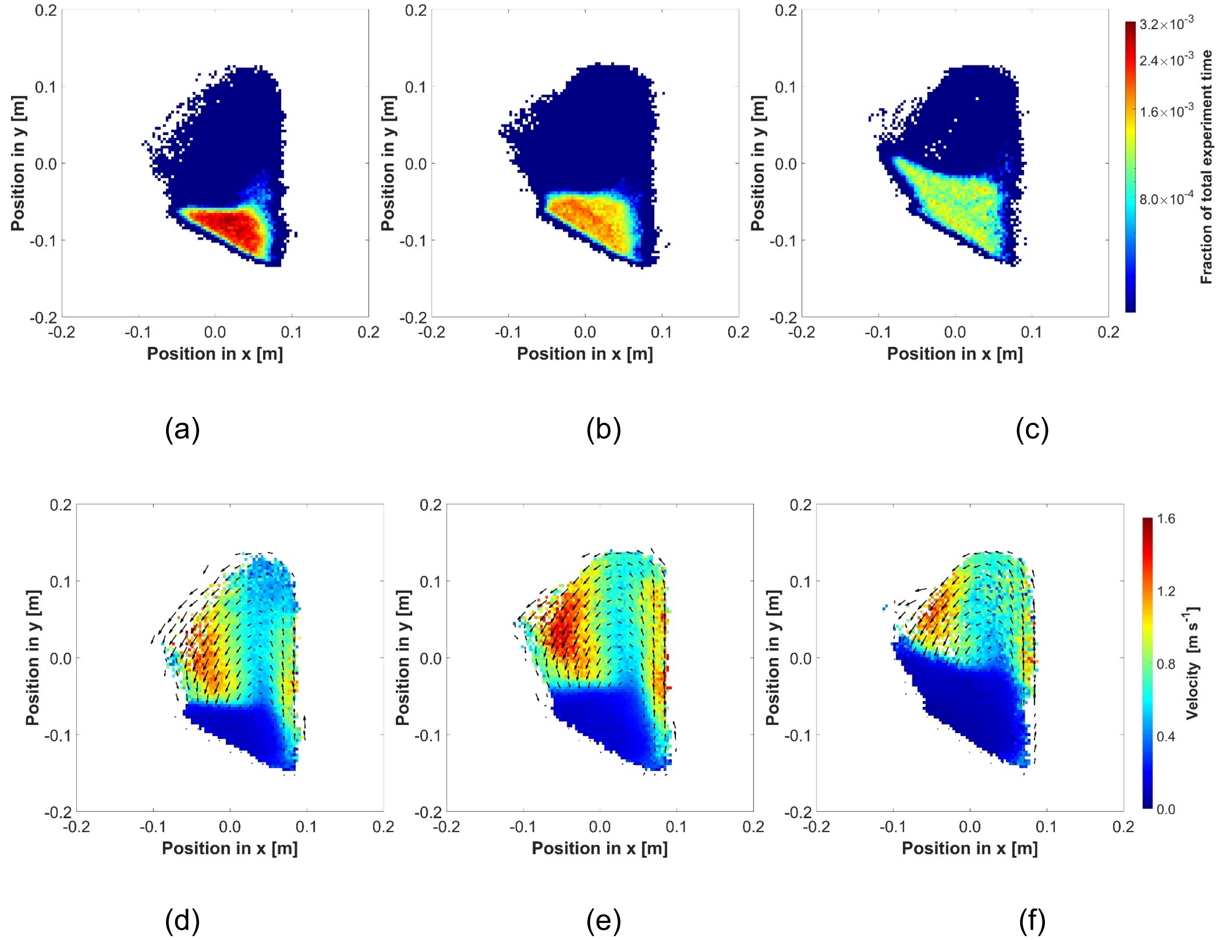

Figure 4. Comparison of (a)-(c) occupancy and (d)-(f) velocity (in plane *xy*) profiles obtained from PEPT data corresponding to batches of 350g of coffee of different density studied at a fan frequency of 48 Hz. Coffee bean densities correspond to: (a) and (d), green; (b) and (e), part-roasted; (c) and (f), roasted coffee.

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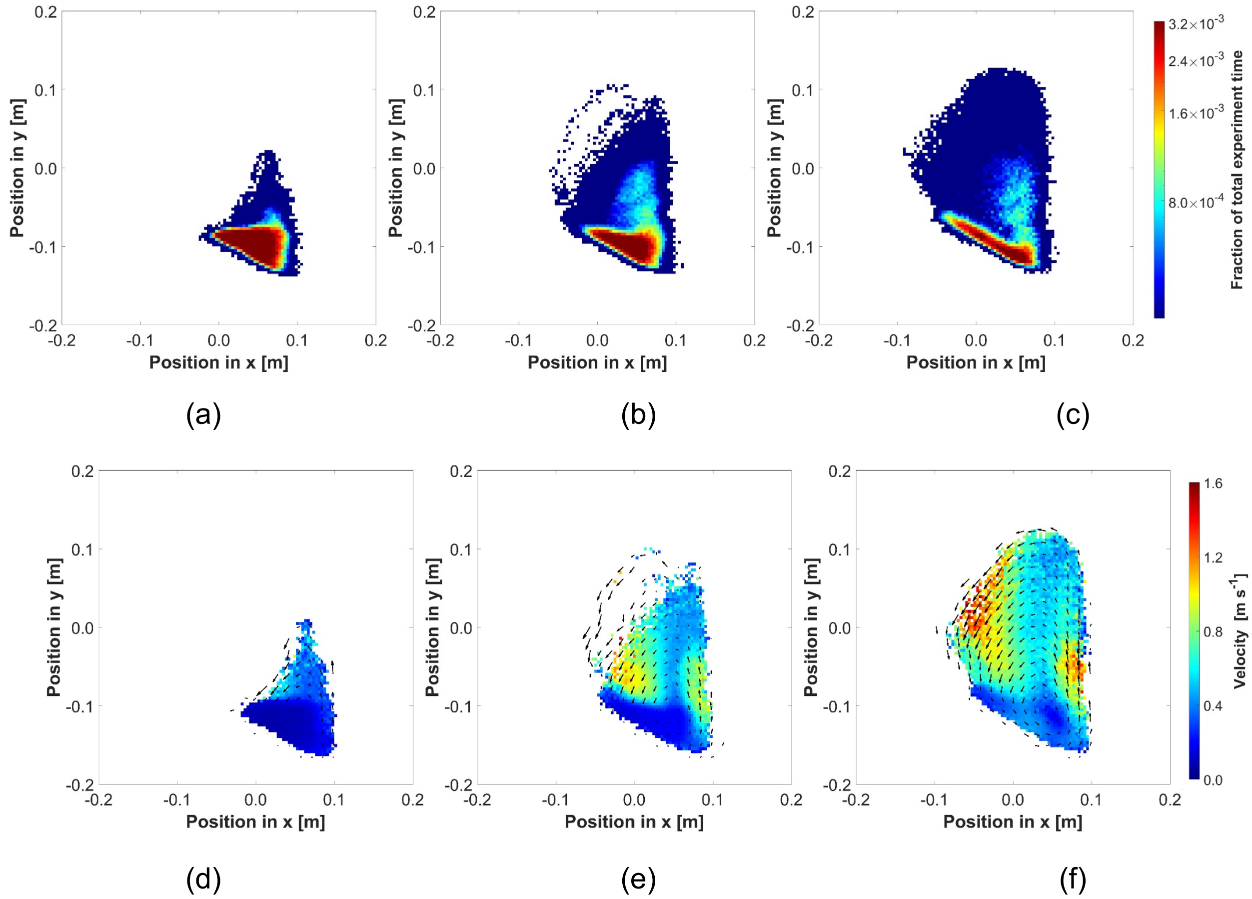


Figure 5. Comparison of (a)-(c) occupancy and (d)-f) velocity (in plane *xy*) profiles for 200g batches of green coffee subject to different airflows. Airflows correspond to fan frequencies of: (a) and (d), 30 Hz; (b) and (e), 48 Hz; (c) and (f), 65 Hz.

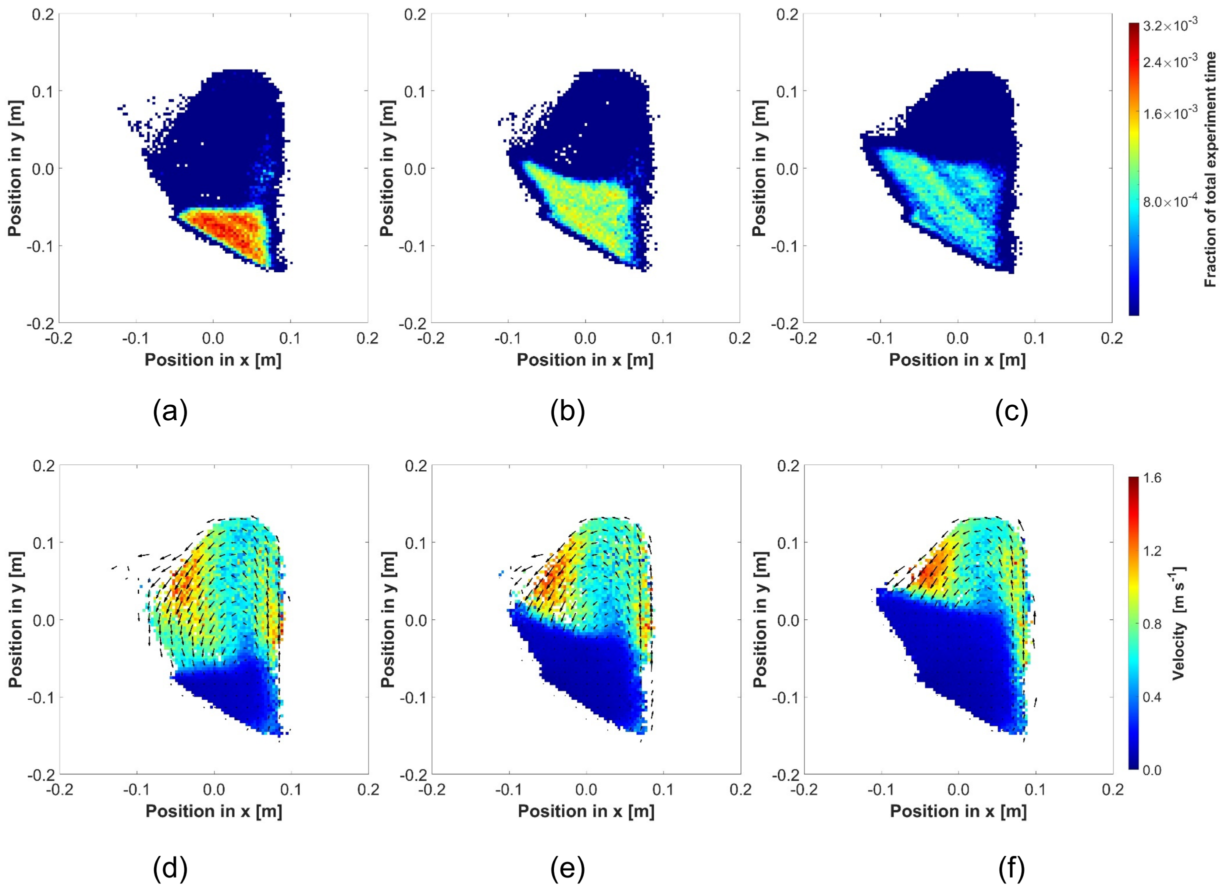
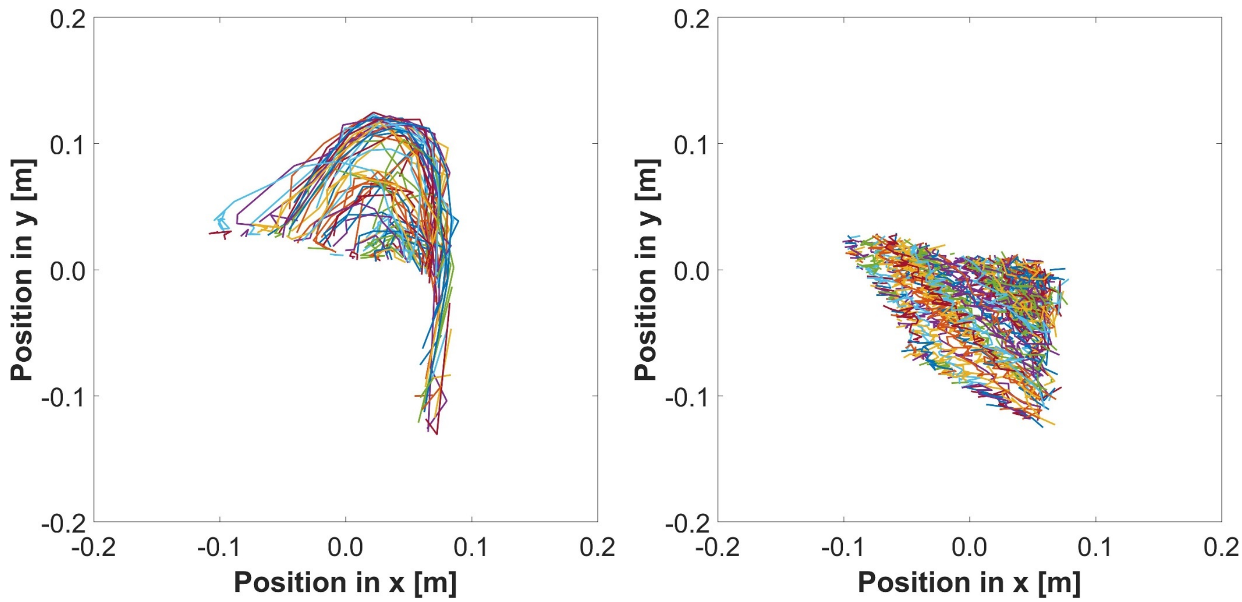


Figure 6. Comparison of (a)-(c) occupancy and (d)-(f) velocity (in plane *xy*) profiles for roasted coffee of different batch sizes subject to air at a fan frequency of 48 Hz. Batch sizes correspond to: (a) and (d), 200g; (b) and (e), 350g; (c) and (f), 500g.



(a) (b)

Figure 7. Particle trajectories of a coffee bean within the a) freeboard and b) bed obtained from PEPT data corresponding to a batch of 500g of roasted coffee subject to moderate airflow (48 Hz). Data is the same as that plotted in Figures 6 (c) and 6 (f).

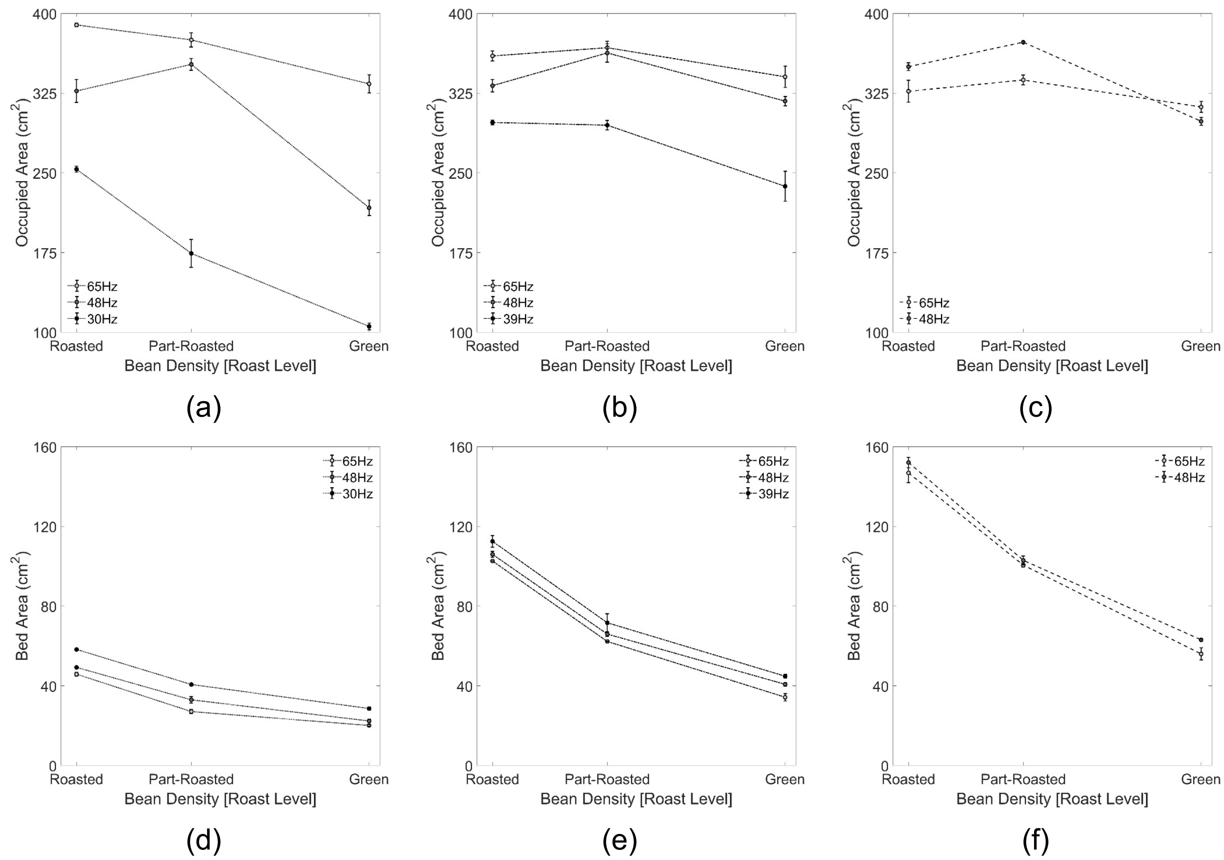


Figure 8. Changes in (a)-(c) occupied area and (d)-(f) bed area as a function of coffee density and airflow for batch sizes of: (a) and (d) 200g; (b) and (e) 350g and (e) and (f) 500g, in plane *xy*.

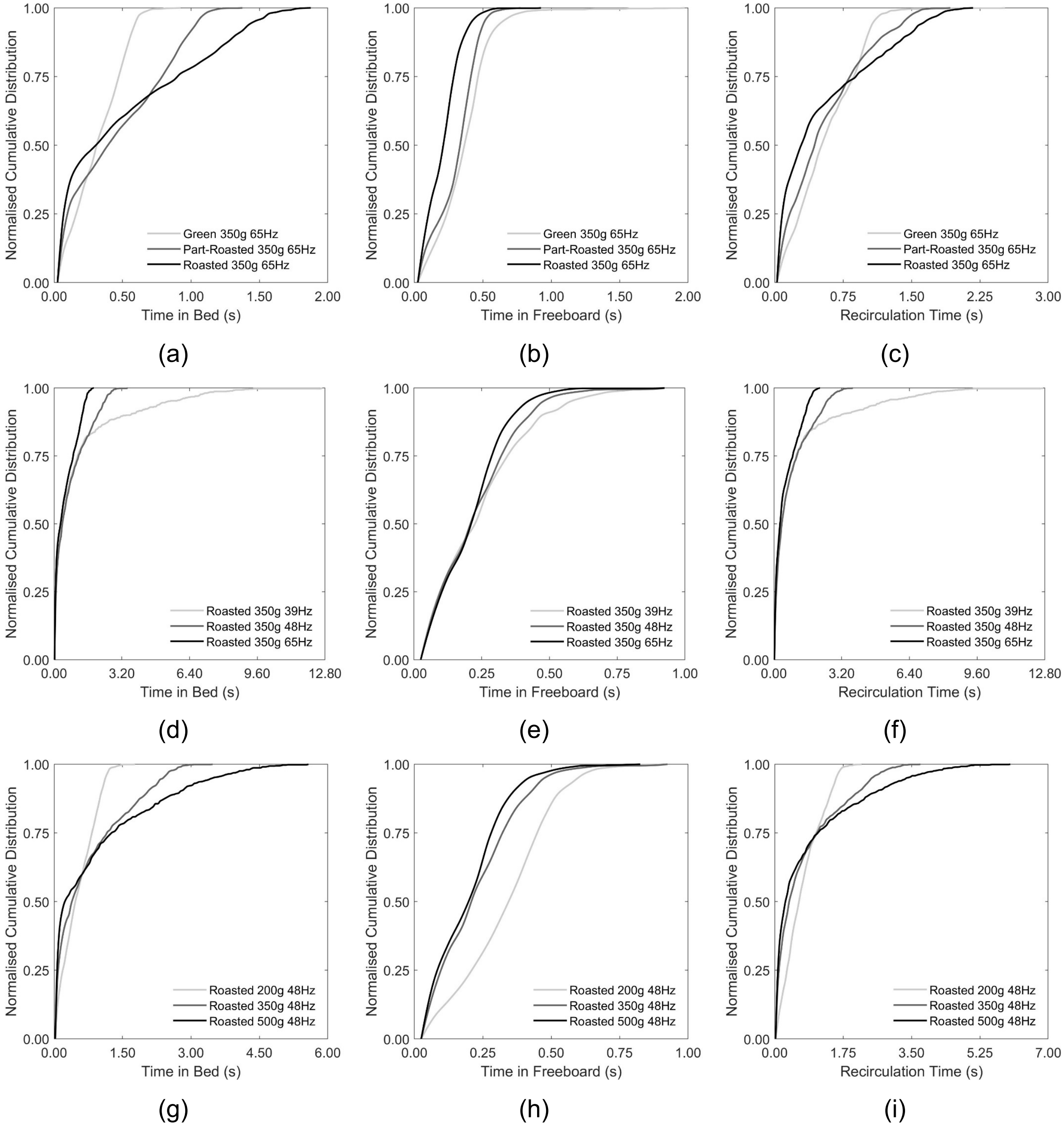


Figure 9. Cumulative distributions of residence time (a), (d) and (g) in the bed, (b), (e) (h) in the freeboard and (c), (f) and (i) from spout-to-spout (i.e., recirculation times, where spout-to-spout residence times are the sum of the freeboard and bed residence times). The effect of coffee density is shown in (a)-(c) for 350g of coffee with different densities subject to high (65 Hz) airflow; the effect of air flow is shown in (d)-(f) for 350g of roasted coffee subject to different air flows; the effect of batch size is shown in (g)-(i) for different batch sizes of roasted coffee at moderate (48 Hz) airflow.

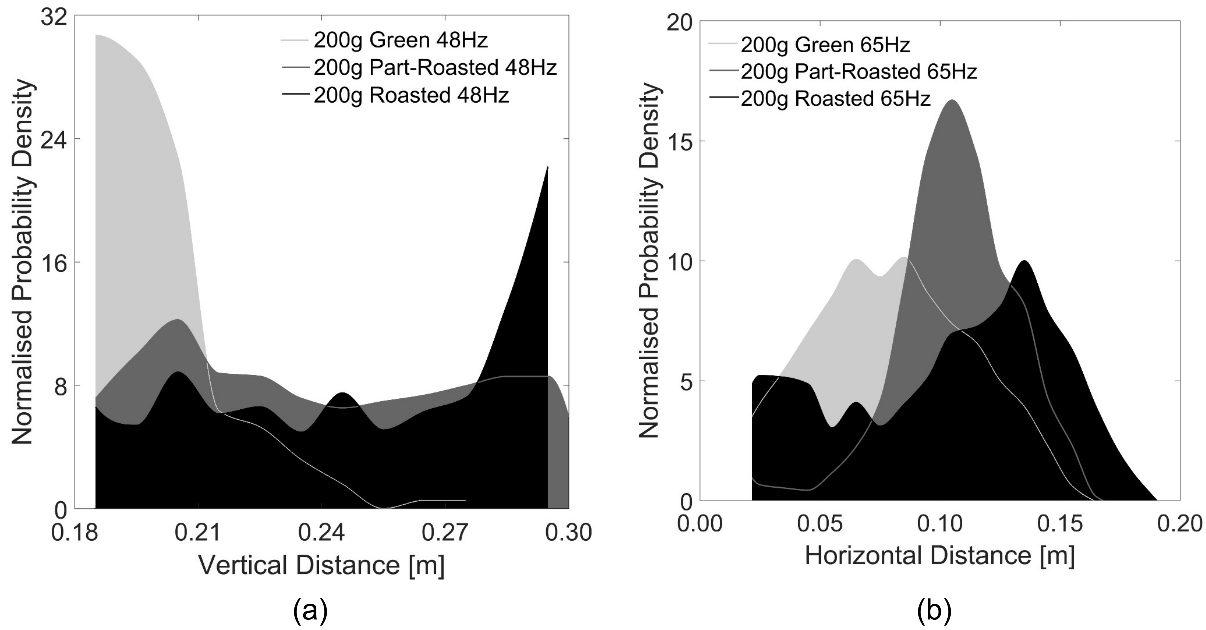


Figure 10. Changes in (a) vertical and (b) horizontal freeboard distances traversed by coffees beans of different densities in a 200g batch at a) moderate (48Hz) and b) high (65Hz) air flow.

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TABLES

Table 1. Properties of Kenyan Arabica coffee beans of different roasting degrees.

Coffee Sample	Roast Time (s)	Roast Loss (%)	Principal Dimension a (mm)	Principal Dimension b (mm)	Principal Dimension c (mm)	Volume (mm^3)	Intrinsic Density (kg m^{-3})	Bulk Density (kg m^{-3})
Green	0	0.0	6.18±0.34	3.84±0.41	8.54±0.62	106±3	1311±12	705±11
Part-Roasted	138	8.1	7.08±0.50	4.42±0.48	9.07±0.83	151±7	844±23	460±9
Roasted	278	16.6	7.64±0.49	4.80±0.44	10.38±0.86	206±5	589±8	301±6

Table 2. Airflow properties of the spouted bed roaster as determined by a hot-wire anemometer.

Fan Frequency (Hz)	Air Velocity (m s^{-1})	Air Mass Flow Rate (kg s^{-1})
30	4.2	0.0141
39	5.7	0.0185
48	7.2	0.0228
65	10.0	0.0310

Table 3. Static bean bed area of coffee beans as affected by batch size and bean density in plane *xy*.

Batch Size (g)	Coffee Sample	Bed Area in *xy* (cm^2)
	Green	28.85±0.42
200	Part-Roasted	44.25±0.87
	Roasted	83.44±2.55
	Green	50.50±0.76
350	Part-Roasted	103.28±3.03
	Roasted	184.71±4.47
	Green	92.67±2.16
500	Part-Roasted	169.65±4.33
	Roasted	285.99±6.39