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Original Article

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Characterization of Naturally Occurring Alpha-Diketone Emissions and Exposures at a Coffee Roasting Facility and Associated Retail Café

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Abstract

Background: Alpha-diketones such as diacetyl and 2,3-pentanedione have been used as artificial flavorings in a variety of industries and are produced naturally when food products such as coffee beans are roasted. Exposure to these compounds has been associated with bronchiolitis obliterans, a rare and severe respiratory disease. In the current paper, we (i) evaluate which steps in the coffee production process are associated with the highest alpha-diketone emissions at a small craft coffee roaster and associated café, (ii) determine the extent to which direct-reading measurements of CO, CO_2, and total volatile organic compounds (VOCs) can serve as lower-cost surrogate indicators for diacetyl concentrations, and (iii) conduct a limited emissions study to quantify the effect that the process variable of roast type has on diacetyl emissions from grinding beans.

Methods: Exposure and area concentration data for diacetyl and 2,3-pentanedione were collected over 4 days of sampling at a single coffee roaster and associated café. Additional measurements of café patrons' exposure to diacetyl were collected in seven other craft roastery/cafes in Seattle, WA. For the emissions experiments, integrated area air samples for diacetyl were collected using sorbent tubes over 30-min intervals for each roast type with the sorbent tubes positioned next to a grinder placed in an exposure chamber. Sorbent tubes were analyzed for alpha-diketones using gas chromatography–mass spectrometry. A photoionization detector (PID) was also used to measure continuous total VOC concentrations at the coffee roastery, and during each grinding experiment.

Results: Diacetyl concentrations in five of the seven personal samples from the craft roastery were above the United States National Institute of Occupational Safety and Health (NIOSH) Recommended Exposure Limit (REL) of 5 ppb as an 8-h time-weighted average (TWA)—and one of the seven personal samples exceeded the NIOSH REL for 2,3-pentanedione—9.3 ppb as an 8-h TWA. Median

What's important about this paper

Alpha-diketones such as diacetyl and 2,3-pentanedione have been used as artificial flavorings in a variety of industries and are produced naturally when food products such as coffee beans are roasted. Exposure to these compounds has been associated with bronchiolitis obliterans, a rare and severe respiratory disease. Results from this observational study showed that coffee production workers at this facility had elevated exposures to diacetyl and 2,3-pentanedione compared to the United States National Institute of Occupational Safety and Health (NIOSH) and American Conference of Governmental Industrial Hygienists (ACGIH) recommended exposure guidelines. Similar to previous studies, these data suggest that processing tasks associated with ground coffee are the biggest contributors to workers' exposure to diacetyl and 2,3-pentanedione. Our results indicate that future research could focus on designing and evaluating effective engineering controls, in the form of local exhaust ventilation, with the goal of reducing alpha-diketone emissions and exposures.

diacetyl and 2,3-pentanedione emissions were highest at the bagging machine followed by the grinder, roaster, barista, and background areas. The arithmetic mean diacetyl concentrations from the seven personal samples collected from café patrons was 3.96 ppb, suggesting that diacetyl exposure poses a negligible health risk to café patrons. Correlations between diacetyl and total VOCs, CO, and CO_2 showed that diacetyl was well correlated with total VOCs, but poorly correlated with CO and CO_2. Based on our limited emissions study, French roast was associated with the highest mass emission factor of diacetyl.

Conclusions: Results from the exposure assessment study indicated that coffee production workers at this facility had elevated exposures to diacetyl and 2,3-pentanedione compared to recommended guidelines, whereas baristas and café patrons received lower exposures. Area sampling showed that the areas with the highest alpha-diketone emissions were the grinder and the bagging machine, which are both areas associated with tasks involving ground roasted coffee. Future research could focus on designing and evaluating effective engineering controls, in the form of local exhaust ventilation, with the goal of reducing alpha diketone exposures, as well as conducting similar studies at other small-scale craft coffee roasters and cafés to better understand the variability in these emissions and exposures within these types of facilities.

Keywords: alpha-diketone; coffee grinding; coffee industry; coffee roasting; diacetyl; exposure monitoring; 2,3-pentanedione; personal exposure

Introduction

Diacetyl and related alpha-diketones are used as artificial flavorings in a variety of foods and beverages to impart a characteristic buttery flavor (McKernan *et al.*, 2016). Diacetyl is also produced in foods naturally as a product of fermentation from bacteria and yeast and via pyrolysis, such as in the roasting of green coffee beans (Shibamoto, 2014; McKernan *et al*, 2016). Prior to roasting, green coffee beans contain "little to no" diacetyl and 2,3-pentanedione (Gaffney *et al.*, 2015). When coffee is roasted at high temperatures (i.e. >200°C), the Maillard reaction takes place wherein amino acids chemically react with sugars to form carbonyl compounds, including diacetyl and other alpha-diketones (Shibamoto, 2014; Tamanna and Mahmood, 2015). Other emission products generated by the roasting process include various VOCs, organic acids, and combustion products, including CO and CO_2 (EPA, 1995). According to the United States Environmental Protection Agency's (EPA's) list of emission factors for coffee roasting operations, for every ton of coffee roasted in a batch roaster, 0.86 lbs of total VOCs and 180 lbs of CO_2 are produced from pyrolysis (EPA, 1995).

The main health endpoint of concern associated with exposure to diacetyl and other alpha-diketones is bronchiolitis obliterans—colloquially referred to as "popcorn lung." Bronchiolitis obliterans is a rare, severe fixed airway disease characterized by inflammation of the small airways of the lungs (bronchioles) leading to irreversible lung damage that may be fatal (NIOSH, 2017). Symptoms of the disease include cough, shortness of breath on exertion, or wheezing, and do not typically improve away from work (NIOSH, 2017). A range of other obstructive lung diseases (e.g. asthma, chronic pulmonary disease, and hypersensitivity pneumonitis) have been associated with exposure to diacetyl in flavorings, but the strength of these associations is weaker than that for bronchiolitis obliterans (SCOEL, 2014).

The United States Occupational Health and Safety Administration (OSHA) has not set standards for the regulation of worker exposure to diacetyl or other alpha-diketones (McCoy *et al.*, 2017). However, the United States National Institute of Occupational Safety and Health (NIOSH) proposed a Recommended Exposure Limit (REL) of 5 ppb for diacetyl as an 8-hr time-weighted average (TWA) and a short-term exposure limit (STEL) of 25 ppb for a 15-min time period (McKernan *et al.*, 2016). Because 2,3-pentanedione is often used as a substitute for diacetyl in flavoring operations and has been demonstrated to cause similar airway epithelial damage, NIOSH also set a REL of 9.3 ppb (TWA) and a STEL of 31 ppb for 2,3-pentanedione (McKernan *et al.*, 2016). The American Conference of Governmental Industrial Hygienists (ACGIH) proposed threshold limit values (TLVs) for diacetyl of 10 ppb (TWA) and a STEL of 20 ppb (ACGIH, 2012).

There is clear evidence from multiple prior studies conducted at commercial coffee roasters that production workers working with unflavored coffee beans have been exposed to diacetyl and 2,3-pentanedione above NIOSH's RELs of 5 and 9.3 ppb, respectively (see Supplementary Table 1, available at *Annals of Occupational Hygiene* online). There is a wide range of variability in exposures to diacetyl both between the different facilities and within the different production areas. This variability may be due to variations in process elements between facilities (i.e. roast temperatures, bean type, and bean origin), the degree of automation present in this facility (i.e. how proximal the worker is to the production process), and whether there are effective ventilation systems or other controls present to reduce worker exposure to diacetyl and other alpha-diketones.

Most of the prior studies have taken place at large or medium-sized roasters; there is limited information on the exposure risk at smaller craft roasters and cafés where production process and worker exposure may differ from the larger facilities. Supplementary Table 1, available at *Annals of Occupational Hygiene* online, summarizes data from prior literature reporting diacetyl exposures and area concentrations in coffee production facilities. LeBouf *et al.* recently published a comprehensive summary of diacetyl measurements in coffee production facilities from a series of Health Hazard Evaluations undertaken by NIOSH (LeBouf *et al.*, 2020). Although a number of authors sampled for total VOCs, CO, and CO_2 in addition to diacetyl at various coffee processing facilities, to date there have been no studies that have reported correlations amongst these four parameters. Total VOCs, CO, and CO_2 can all be measured with direct-reading instruments in contrast to alpha-diketones, which are measured with sorbent tubes requiring laboratory analysis. Sampling for alpha diketones can be expensive and time-consuming. In contrast, direct-reading instruments deliver data in real-time with minimal per-sample cost after the initial purchase of the instrument. This paper aims to extend prior research by examining exposure to and emissions of diacetyl and other alpha-diketones among workers in a small craft coffee roaster and associated café, examining exposure to diacetyl among café patrons at other craft roasteries/cafés, determining the extent to which direct-reading measurements of CO, CO_2, and total VOCs can serve as lower-cost surrogate indicators for diacetyl concentrations, and quantifying emissions from grinding a variety of different roasts to determine if this process variable has an impact on diacetyl emission factor per mass of coffee ground.

Methods

The study involved three components: (i) assessment of coffee production workers' exposure to diacetyl, conducted in a small craft coffee roastery; (ii) assessment of café patrons' exposure to diacetyl, conducted in seven retail roastery/cafés; and (iii) laboratory study of determinants of diacetyl emissions from grinding of coffee.

Coffee production workers' exposure study

The craft roastery study site consists of green bean storage and roasting room, grinding and packaging room, retail café and seating area, an office and other storage areas. The facility can process coffee beans up to 42 kg/h (~93 lbs/h). Over 4 days of sampling, the median mass of coffee roasted per day was 169 kg (range: 152–250 kg) or approximately 372 lbs per day (range: 336–552 lbs)

The roastery staff includes a primary, experienced operator (the owner), who is assisted by one or two staff when production increases in the fall season. During the survey, the operator intermittently was assisted by one staff member in the roastery. Café operations are typically managed by two to three baristas that take orders and make food and beverages. Many of the beverages made at the café consist of espresso shots, which require the barista to grind and brew espresso beans at the counter.

In the roasting room, green Arabica coffee beans are added to a roaster (Diedrich Roaster IR-12) in approximately 12 kg (~24 lbs) batches. Depending upon the blend, the roast temperature varies from 355 to 480°F (179–249°C), and the roast time varies from 16–18 min. When the roasting cycle is complete, the roasted beans are dropped into the roaster's cooling tray to cool for about 2 min. The roasted beans are then transferred to plastic totes, which are manually carried into the adjacent grinding and packaging room. After three or four batches of beans from different origins (e.g. Columbian, Sumatran, Ethiopian, and so on) are roasted, the roasting operator manually mixes the different beans together for one to two minutes to produce the desired coffee blend.

The roasted beans are either ground and packaged or packaged as whole beans. To grind and package beans, roasted beans are manually scooped from the totes and dumped into one of two Grindmaster grinders. The ground beans are collected in bags and transferred into a bulk scale bagging machine (Logical Machines model S5). This machine weighs bags of whole or ground beans at preset weights of 0.75, 1, and 5 lbs (0.34, 0.45, and 2.27 kg). Bags of ground or whole coffee beans are stored in the grinding and packaging room in polyethylene bags fitted with a one-way valve that allows the roasted coffee to off-gas but does not allow outside air to enter.

The roasting room has an approximate volume of 4000 ft^3 (~113 m^3). The adjacent grinding/packaging room has an approximate volume of 5000 ft^3 (~142 m^3). General ventilation is provided in the roasting room through a ceiling-mounted vent and rooftop blower. The roaster draws air through its after-burner and exhaust system, which provides effective capture and removal of the volatile compounds generated during the roasting process. Additionally, the roaster's cooling tray is equipped with down-draft ventilation that draws air through the tray to facilitate the removal of chaff from the beans (Diedrich, 2017).

Data collection at the roastery/café consisted of four days of sampling on consecutive Tuesdays and Wednesdays in mid- to late-October 2019. Samples were collected from 7:00 am to 3:00 pm on each sampling day, corresponding to the full-shift roasting, grinding, and packaging operations in the roastery. At the beginning of each sampling day, sampling equipment was set up in the barista area, behind the shelves in the café, next to the roaster, and next to the bagging machine. The area samples behind the shelves in the café were intended to capture the background concentrations of alpha-diketones present in this facility. Due to equipment constraints, sampling equipment next to the bagging machine was moved next to the grinders halfway through the day to obtain area samples from the grinding process. The fixed location sampling equipment was placed at approximately breathing zone height and as close as possible to the production tasks being performed. Personal sampling equipment was placed on workers at the start of their shift, and sampling was paused while the workers went off-site for deliveries or took breaks. A total of seven personal samples were taken from two workers across the four days of sampling.

Diacetyl and 2,3-pentanedione were collected on silica gel sorbent tubes (SKC Inc., P/N 226-183) using OSHA methods 1013/1016. In accordance with the methods, two sorbent tubes were connected in series for each sample (OSHA, 2008, 2010). GilAir Plus (Sensidyne, LP) personal air sampling pumps set at 50 ml/min using a Bios DryCal Defender 510 primary flow meter (Mesa Labs, Inc.) were used for both personal and area air samples. The pumps were calibrated before and after each sampling event. After the samples were collected, the tubes were immediately wrapped in aluminum foil and refrigerated until extraction.

Two photoionization detectors [PIDs; MiniRae 3000 PID (RAE Systems, Inc.) and a Photovac 2020ppb PRO Photoionization Monitor (Photovac, Inc.)] were deployed to measure continuous total VOC (TVOC) concentrations at the roasting, grinding, and packaging stations. The probes of the PIDs were positioned next to the respective production machines (i.e. roaster, grinder, bagging machine) at approximate breathing zone height and were positioned to be facing towards the work activity being performed. Tygon tubing was used to extend the length of the probe for the PID positioned next to the bagging machine. Due to problems with logging data, TVOC data were only available at the grinder and bagging machine location for three of the four sampling days.

CO and CO_2 concentrations were measured at the roasting, grinding, and packaging stations using two Indoor Air Monitors (TSI Q-Trak Model 7575). The probes of the Q-Traks were positioned next to the respective production machines at approximate breathing zone height and were positioned to be facing toward the work activity being performed. Due to problems with logging data, CO, and CO_2 data were only available for three of the four sampling days.

In addition, daily task observation forms were completed for the production area. A study team member would observe the roastery workers as they roasted, ground, and bagged coffee beans and would record the start and stop times of each activity for the duration of the sampling day. The observer would note when each batch of coffee began roasting and when the roasted beans dropped into the cooling tray. They would also note when grinding or bagging was taking place and which worker was performing those activities.

Café patrons' exposure study design

A standardized protocol to measure potential diacetyl exposures of café patrons was used. A study team member visited seven craft roaster/cafés where they would enter the café, order an 8 oz latte, sit at a private table in close proximity to the barista area, and consume the latte at a standard rate during a 90-min period. The researcher wore a sorbent tube in the personal breathing zone to sample for diacetyl, as described previously, except that the sampling rate was set to 200 ml/min. The sampling pump was started as soon as the researcher sat down at the table and was terminated 90 min later.

Emissions study design

The purpose of the laboratory study was to quantify the diacetyl emissions from various types of coffee roasts during grinding. White coffee (light roast), medium espresso, espresso, and French roast were purchased from the roastery where the coffee production workers' exposure study took place. White coffee is the lightest roast out of the four and is roasted at 355°F (~179°C). The medium espresso is roasted at 458°F (~237°C) and the espresso is roasted at 468°F (~242°C). The French roast is the darkest roast out of the four and is roasted at 475°F (~246°C). The roastery uses only Arabica coffee, and the espresso blends include Central American, South American, and Indonesian coffee beans.

Emissions tests were conducted in a Plexiglas emissions test chamber (volume 189 l) located at the University of Washington. A Grindmaster industrial coffee grinder was placed inside the experimental chamber together with a small fan to ensure that air in the chamber was well-mixed. The chamber had a sealed glove bag attached to it that allowed the user to remove the coffee grounds during the experiment. A MiniRAE 3000 PID (RAE Systems, Inc.) was placed inside the chamber to measure total VOC emissions during grinding. Diacetyl was collected on silica gel sorbent tubes as described previously, at a sampling rate of approximately 200 ml/min. The sorbent tube samples were co-located with the MiniRAE's sampling probe in the chamber. A high-volume air pump was attached to the chamber and drew air from outside the chamber through the system at a rate of 30 l/min. The pump was pre- and post-calibrated for each set of experiments and initial and final chamber flow rates were averaged to obtain the average chamber flow rate for each trial.

For each trial, 8 oz (approximately 227 g) of coffee beans were ground in the sealed experimental chamber, which took approximately 30 s. The grinder continued to operate for 5 min after the grinding was completed to mimic the process utilized at the coffee roastery where fieldwork was conducted. The grounds were then removed from the chamber via the glove bag. Each trial ended after 30 min had passed from the start of grinding. Each experiment consisted of three trials. To verify that there was no diacetyl and minimal TVOCs in the room air and chamber, two sets of experimental blanks were obtained for each experiment by running the entire experiment without adding coffee to the system. One experimental blank was collected before any coffee grinding was done and one blank was collected after all coffee grinding was completed. Diacetyl levels measured in the post-experiment blanks were on average 3.7% of diacetyl levels measured during the grinding experiments. Furthermore, diacetyl levels measured in the post-experiment blanks did not increase from one experiment to the next. These data indicate that losses of diacetyl due to adsorption to the walls of the Plexiglass chamber were negligible.

Sample analysis

Diacetyl and 2,3-pentanedione sample analysis

Diacetyl and 2,3-pentanedione were analyzed according to OSHA Methods 1013/1016 with some modifications (LeBouf, 2017; OSHA, 2008, 2010). The sorbent from each sample's front and back tubes was transferred into separate labeled 4 ml amber vials and the filter and front and back glass wool from the tubes were discarded. 2 ml of 5% methanol/acetone containing 2.5 μl/ml of internal standards (ISTD) 2,3-butanedione-d^6 and 25 µl 2,3-pentanedione-1,1,1,4,4-d^5 were added to each vial for extraction. Samples were extracted on a rotator for 60 min and an approximate 200–300 μl aliquot of the solution was then transferred to a 1.8 ml amber gas chromatography vial with the remainder stored at –20°C. The samples were analyzed using gas chromatography–mass spectrometry (GC/MS Agilent 7890B/7000, Santa Clara, CA). Analyte recoveries were determined by analyzing sorbent tubes spiked with diacetyl and 2,3-pentanedione and varied between 89% and 98%. Calibration standards in the range 0.6–1200 ng/ml were analyzed, and calibration curves were calculated using linear regression (R^2 > 0.99) and applied to calculate analyte concentrations in the air samples collected. The limit of detection was 1 ng for both analytes. Analyte concentrations were determined by adding the mass of each compound on the front and back tubes then dividing by the total volume of air that was sampled. Analyte mass on the back tube was less than 10% of the analyte mass on the front tube, indicating that no significant sample loss due to breakthrough occurred under the specific sampling conditions.

Emission factors were determined by adding together the mass of diacetyl on the front and back tubes, then multiplying this value by the ratio of the total air volume pulled through the chamber, divided by the air volume pulled through the sorbent tube. This product was then divided by the mass of coffee ground per experiment to get the mass emission factor in units of ng diacetyl per gram of ground coffee.

Statistical analysis

Diacetyl and 2,3-pentanedione concentrations were calculated for each day of sampling based on two exposure scenarios. The first assumed zero exposure for the remainder of the 8 h because in most cases the employee was finished with coffee processing tasks for the day. The second scenario assumed that there was steady exposure for the remainder of the 8 h and would represent a TWA exposure if the worker were to continue their coffee production tasks for a full eight hours. Summary statistics for diacetyl and 2,3-pentanedione concentrations measured at each sampling location were calculated, and boxplots were created to visualize analyte concentrations at each sampling location.

Microsoft Excel software was used to create simple linear regression models that correlated median CO, CO_2, or total VOC concentrations measured at each sampling location to corresponding median diacetyl concentrations measured at that same location. 95% confidence intervals for predicted average diacetyl concentrations at specified total VOC concentrations were created using the "predict" function in R Studio software (R Core Team, 2017).

Diacetyl mass emission factors were calculated for each set of grinding experiments and these values were compared across the different roast types. Using R Studio software, a one-way ANOVA test with a significance level of $\alpha = 0.05$ was utilized to determine if there was a significant overall difference in mean diacetyl mass emission factors by roast type (R Core Team, 2017). Conditional on the ANOVA test showing significant differences, post-hoc Tukey HSD pairwise comparisons (with a Bonferroni-adjusted significance level of $\alpha = 0.01$) of the mean diacetyl concentration for each roast type were carried out to determine significant differences in mean diacetyl emission factors between specific roasts.

Results

Coffee production workers exposure study

Table 1 summarizes the personal exposures measured on the production workers. Assuming zero exposure for the remainder of the 8 h, the median diacetyl exposure was 9.1 ppb (range = 1.0–21 ppb), and the median 2,3-pentanedione exposure was 4.8 ppb (range = 0.5–11 ppb). Full-shift diacetyl exposures frequently exceeded NIOSH and ACGIH 8-h exposure limits, with five of seven samples exceeding the NIOSH REL and three of seven samples exceeding the TLV (Table 1). One 4-h sample also exceeded the ACGIH short-term exposure level (STEL) for diacetyl (20 ppb) with an exposure of 21 ppb. One 2,3-pentanedione exposure exceeded the NIOSH 8-h REL, but none exceeded the NIOSH STEL.

Assuming steady exposure to diacetyl and 2,3-pentanedione for the remainder of an eight-hour shift, six of seven samples would have exceeded the NIOSH 8-h REL for diacetyl and five of seven samples would have exceeded the TLV (Table 1). One 4-h sample

Table 1. Diacetyl and 2,3-pentanedione personal exposure results.[a]

	Sample Duration (min)	Diacetyl no exposure[b] 8-h TWA (ppb)	Diacetyl steady exposure[c]* 8-h TWA (ppb)	2,3-Pentanedione no exposure 8-h TWA (ppb)	2,3-Pentanedione steady exposure[c]* 8-h TWA (ppb)
Median (minimum–maximum)	329 (148–408)	9.1 (1.0–21.0)	16 (1.5–32)	4.8 (0.5–11)	6.9 (0.7–17)

[a]Sample size ($N = 7$).
[b]8-h TWA exposure assuming zero exposure for the remainder of the 8 h.
[c]8-h TWA exposure assuming steady exposure for the remainder of the 8 h.
*Actual personal exposure determined over the sample duration.
NIOSH REL: 5 ppb for diacetyl; 9.3 ppb for 2,3-pentanedione.
ACGIH TLV: 10 ppb for diacetyl.

also would have exceeded both STELs for diacetyl (20 and 25 ppb, respectively) with an exposure of 39 ppb. Three of seven samples would have exceeded the NIOSH 8-hour REL for 2,3-pentanedione, but none would have exceeded the NIOSH STEL.

Overall, 2,3-pentanedione exposures were less than diacetyl exposures by approximately 50–70%. On days where workers were doing more grinding and packaging of ground beans, their exposures to diacetyl and 2,3-pentanedione were higher compared to days where they were doing less grinding and packaging.

Diacetyl and 2,3-pentanedione concentrations were highest at the bagging machine, followed by the grinder, roaster, barista, and background areas (Fig. 1). Area measurements of diacetyl and 2,3-pentanedione collected in the barista and café were consistently below exposure guidelines, indicating that exposure of café workers and customers were below levels of concern. In contrast, median concentrations of diacetyl and 2,3-pentanedione at the bagging machine and the grinder exceeded both exposure guidelines, and concentrations of diacetyl at the roaster exceeded the NIOSH REL. These data suggest that workers near the bagging machine and the grinder are at risk to be exposed to hazardous levels of diacetyl and 2,3-pentanedione, consistent with our measurements of exposure on the two roastery workers, which were described above.

Table 2 summarizes concentrations of CO, CO_2, and TVOC at each sampling location. TVOC area concentrations were highly correlated with diacetyl (Fig. 2; R^2 = 0.95, P-value = 4.8 × 10^{-15}), however diacetyl concentrations were less well correlated with CO_2 (Fig. S1, R^2 = 0.58, P-value = 0.001) and CO (Fig. S2, R^2 = 0.09, P-value = 0.34). Moreover, when the relationship between air concentrations of diacetyl and TVOCs is considered by sampling location, the relationship was similar for the two areas with the highest emissions—the packaging area and the grinding area.

Café patrons exposure results

The average diacetyl exposure measured in the seven personal café samples was 3.96 ppb (range 1.1–7.8 ppb). These concentrations were considerably lower than those observed in the production area of the roastery (8–170 ppb) and were similar to levels observed in the barista area of the café associated with the roastery (3.1 ppb).

Emissions study results

Fig. 3 shows an example annotated time-series plot of continuous TVOC concentrations inside the chamber. Based on these time-series plots of continuous TVOC concentrations inside the chamber, it was determined that after 30 min from the start of grinding, greater than 90% of emissions had been evacuated from the chamber.

We found that French roast was associated with the highest mass emission factor of diacetyl (median: 1532 ng diacetyl per gram of coffee ground, range:

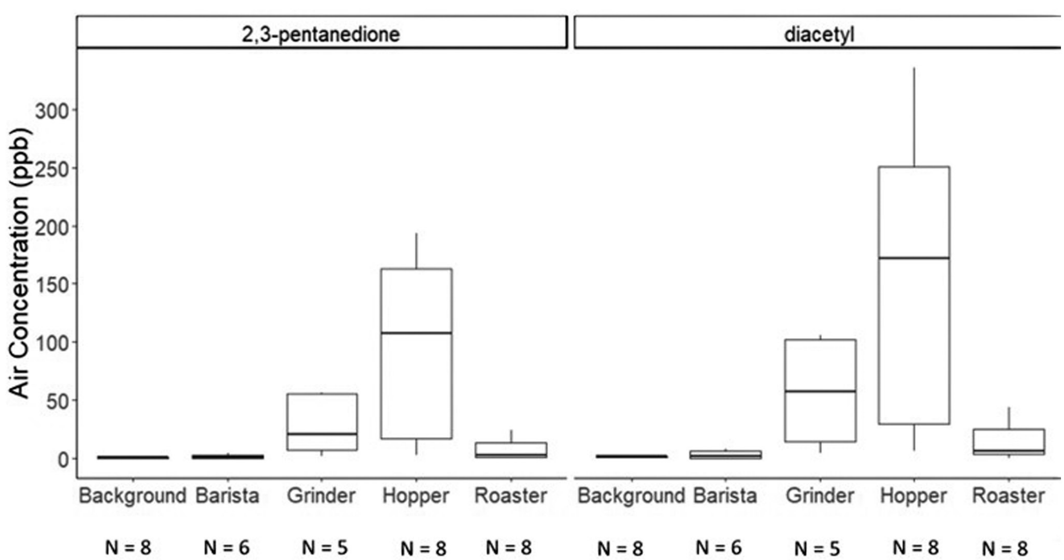

Figure 1. Box plot comparing diacetyl and 2,3-pentanedione concentrations by sampling location. The centerline in each box represents the median value, the lower and upper borders of the box represent the 75th and the 25th percentiles, and the whiskers extend to the largest or smallest value, at most 1.5 × IQR (interquartile range) beyond the box borders.

Table 2. Summary of CO, CO_2, and total VOC (TVOC) area concentrations.

Analyte concentration median (minimum–maximum)	Roaster	Grinder	Bagging machine	Barista	Background
CO (ppm)	**13.1** (1.6–14) *N* = 6*	**16.4** (<LOD–28) *N* = 3	**17.6** (1.8–22) *N* = 3	NM**	NM**
CO_2 (ppm)	**801** (470–840) *N* = 6	**711** (580– 970) *N* = 3	**1100** (910–1100) *N* = 3	NM**	NM**
TVOC (ppb)	**65** (20–420) *N* = 6	**3400** (1100–3600) *N* = 3	**7000** (1300–9300) *N* = 2.5	**<LOD** *N* = 0.5	**<LOD** *N* = 3

* *N* = # of half-days of sampling. ** Not measured.

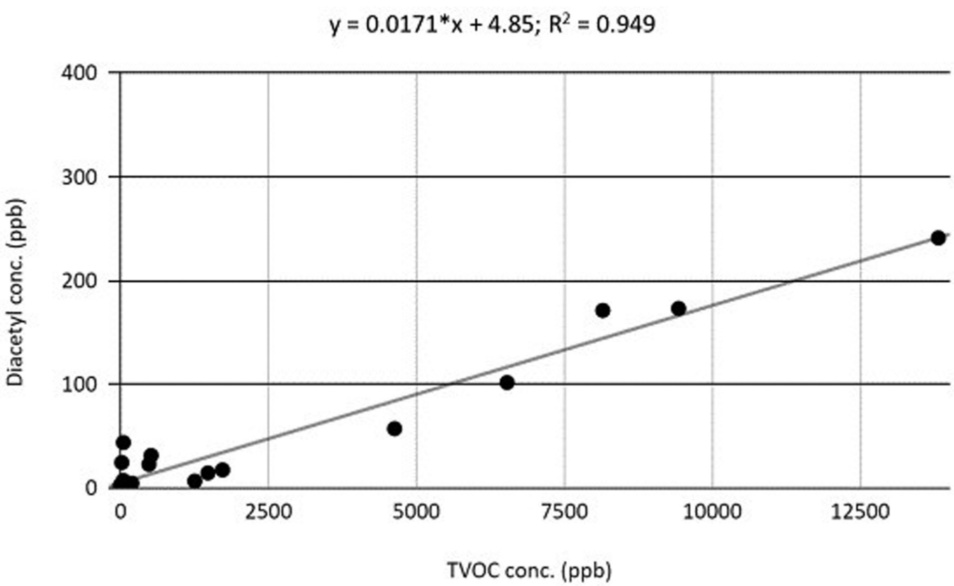

Figure 2. Scatterplot showing a correlation between total volatile organic compounds and diacetyl air concentrations measured at all sampling locations.

1520–1784 ng diacetyl/g of coffee ground), followed by medium espresso (median: 1022 ng diacetyl/g of coffee ground, range: 894–1256 ng diacetyl/g of coffee ground), espresso (median: 879 ng diacetyl/g of coffee ground, range: 844–994 ng diacetyl/g of coffee ground), and white coffee (median: 44 ng diacetyl/g of coffee ground, range: 41–44 ng diacetyl/g of coffee ground) (Fig. 4). The median diacetyl mass emission factor of French roast was almost two times that of espresso, 1.5 times that of medium espresso, and 35 times that of white coffee. The arithmetic mean diacetyl mass emission factor for French roast was significantly higher than those for espresso, medium espresso and white coffee. The arithmetic mean diacetyl mass emission factor for white coffee was also significantly lower than espresso and medium espresso. There was no significant difference between mean diacetyl mass emission factors for espresso and medium espresso.

To further investigate the utility of TVOC measurements as a surrogate for diacetyl, we compared TVOC emission factors to the diacetyl emission factors. We observed a high correlation (0.94) between these two measures. We then used the TVOC data to predict diacetyl emission factors. Linear regression of the TVOC-predicted vs observed diacetyl emission factors yielded a slope of 0.90, indicating that the TVOC data modestly underpredicted the actual diacetyl emission factors in the grinding experiments.

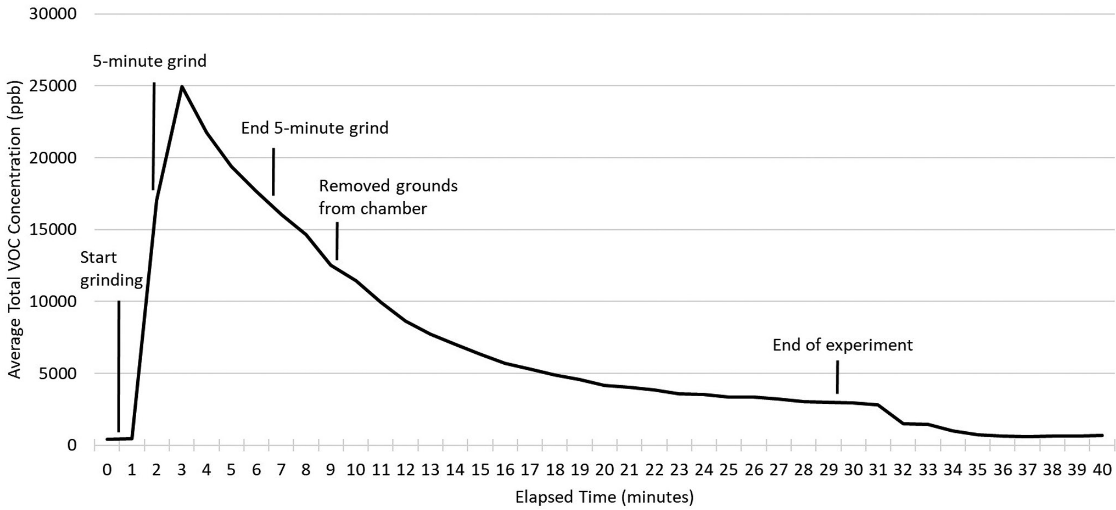

Figure 3. Example time-series analysis plot of the continuous concentration of TVOCs inside the chamber during one trial of the range-finding experiment. After 30 min passed from the start of grinding, over 90% of the emissions generated from grinding had evacuated the chamber

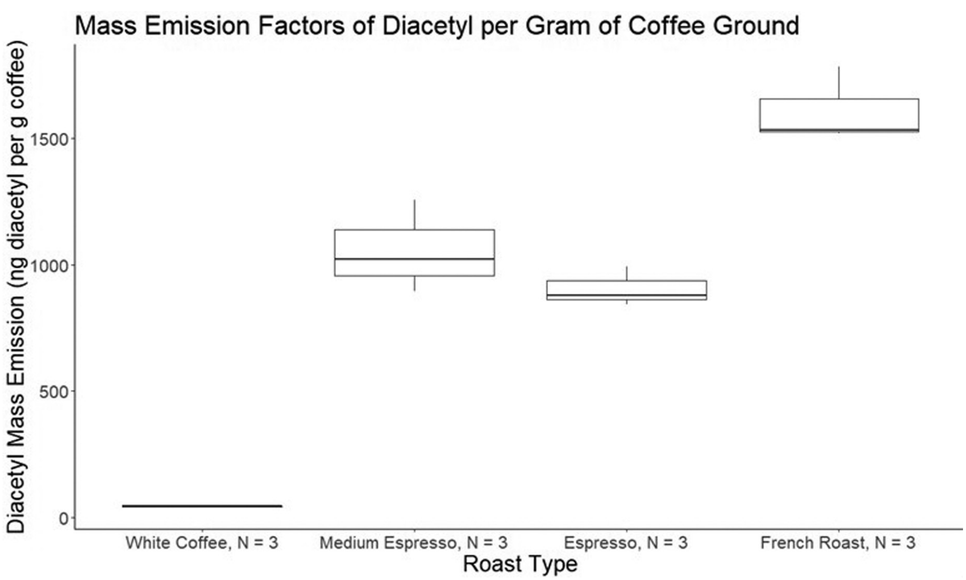

Figure 4. Box plot comparing diacetyl mass emission factors for grinding of each roast type. The centerline in each box represents the median value, the lower and upper borders of the box represent the 75th and the 25th percentiles, and the whiskers extend to the largest or smallest value at most 1.5 × IQR (interquartile range) beyond the box borders. For each roast type, each experiment consisted of three trials.

Discussion

The exposures of coffee production workers at this facility to diacetyl and 2,3-pentanedione frequently exceeded NIOSH and ACGIH recommended exposure guidelines. Harvey *et al*. reported that coffee production workers with similar exposures to those we observed (LeBouf, 2020) had a higher incidence of asthma and reported a greater frequency of ocular, nasal and respiratory symptoms compared to the general US population (Harvey, 2020). Similar to previous studies, diacetyl, and 2,3-pentanedione emissions were highest in coffee bean production areas where activities involved grinding roasted beans or packaging ground roasted beans. A UK study at a large-scale coffee roaster found that the grinding area was associated with the highest average diacetyl air concentration (252 ppb over four 40-min samples) (Table S1), followed by the packaging area (55 ppb over two 30–40-min sample), and the roasting area (13 ppb over five 40-min samples) (Pengelley *et al.*, 2019). A NIOSH study at a small-scale coffee roaster found that air concentrations of diacetyl during short-term sampling were highest for tasks involving grinding roasted beans (maximum: 31.7 ppb) (Hawley *et al.*, 2018). Another NIOSH study conducted at two cafés associated with a small-scale roaster found that diacetyl concentrations in the air measured during short-term task-based sampling were higher for tasks involving grinding of roasted beans (maximum: 125 ppb) (McClelland *et al.*, 2019). Grinding roasted beans increases the surface area for off-gassing of these volatile organic compounds (VOCs) (Akiyama *et al.*, 2003; Gaffney *et al.*, 2015; Blackley *et al.*, 2019). Furthermore, in our study exposure appeared to increase on days where workers were spending more time on tasks involving ground roasted coffee (i.e. grinding and packaging ground beans) compared to days where workers were handling mainly whole roasted beans. For example, workers ground coffee for about an hour total on 29 October and packed only whole beans for about 3.5 h total, whereas on 15 October workers ground coffee for about 3 h total and packaged only ground beans for about 3.5 h (Table S2). These differences in the amount of time spent on production activities and the type of product being processed (i.e. whole versus ground beans) may explain why diacetyl and 2,3-pentanedione exposures were much higher on 15 October than they were on 29 October. Alternatively, the inter-day variability in exposures could also reflect natural variability in work patterns and behaviors. In their study summarizing emissions and exposures of alpha-diketones in 17 coffee roasting and packaging facilities, LeBouf *et al.* found that in facilities that produced unflavored coffee, grinding and moving ground coffee were associated with the highest short-term, task-based exposures to diacetyl and 2,3-pentanedione (LeBouf *et al.*, 2020). These results suggest that efforts to reduce coffee production workers' exposures to these compounds should focus on the process elements where workers are handling ground beans.

The results from the café patron study and the barista/café measurements at the craft roaster are similar to prior literature measurements of barista exposures. Pengelly *et al.* reported personal full-shift 8-h TWA diacetyl exposures measured from three baristas ranged from 0.1 to 0.2 ppb (Pengelly *et al.*, 2019). In their summary of data from NIOSH HHEs, LeBouf *et al.* reported a geometric mean diacetyl exposure of 4.1 ppb for baristas (LeBouf *et al.*, 2020). Higher exposures were recorded from a NIOSH study conducted at two cafés associated with a small-scale coffee roaster, which found that full-shift 8-h TWA diacetyl exposures measured on a barista at one café ranged from 5.1 to 5.8 ppb, and full-shift diacetyl exposures measured on a barista at the second café ranged from 3.3 to 13.9 ppb (McClelland *et al.*, 2019). A literature search identified no prior published studies where coffee shop patron's diacetyl exposures were determined. Although our study represented a scripted scenario designed to emulate the diacetyl exposures that might be experienced by a café patron, the low exposures we observed, together with the fact that café patrons would typically experience durations of exposure much shorter than 8 h upon which the NIOSH TWA REL is based, indicate that diacetyl exposures are of minimal health risk for café patrons.

A strong correlation between area measurements of TVOCs and diacetyl concentrations ($R^2 = 0.95$) in the roaster was observed. This relationship was also noted in the laboratory emissions measurements (data not shown). We were interested in using TVOC measurements as a surrogate for diacetyl concentrations, as a measurement of diacetyl is challenging and costly. However, despite the high correlation we observed between TVOC and diacetyl, there was a substantial error in using TVOCs measurements to predict diacetyl concentrations at levels close to the REL. Using a regression model constrained to diacetyl concentrations <100 ppb, a TVOC concentration of 100 ppb corresponds to a diacetyl concentration of 7.1 ppb (95% confidence interval: 1.5–12.6 ppb). The wide confidence intervals generated by this model make it impractical for reliably estimating whether diacetyl exposures exceed exposure guidelines. Potential explanations for the poor precision of these predictions include (i) insufficient measurements close to the REL to reliably calibrate the prediction model, (ii) spatial variability between collocated diacetyl and TVOC samples, and (iii) the accuracy of the direct-reading instruments is poorer at the lower end of their measurement range.

In the laboratory study, we found that French roast was associated with the highest mass emission factor of diacetyl, followed by medium espresso, espresso, and white coffee. Roasting temperature is an important determinant of diacetyl emissions with emissions from white coffee being significantly lower than the darker roasts. Similarly, LeBouf and Aldrich recently reported that CO emissions from ground coffee beans were higher for darker roasts compared to lighter roasts (LeBouf and Aldrich, 2019). However, diacetyl emissions were substantial for all types of darker roasts, so minimizing diacetyl formation by lowering roasting temperatures is not a feasible approach to reduce worker exposures. For smaller operations that do not engage in 40-h per week of processing activities distributing the roasting, grinding, and bagging activities more evenly throughout the week could greatly reduce the daily TWA alpha-diketone exposures and improve compliance with NIOSH and ACGIH recommended health guidelines. Whether that approach would impact worker health depends on whether peak exposures matter more than cumulative exposures. NIOSH recommended STELs for diacetyl and 2,3-pentanedione based on the concern that peak exposures may have greater toxicity than the same dose spread out over a longer period of time, albeit this recommendation was based on limited data obtained from animal studies (McKernan *et al.*, 2016). The use of local exhaust ventilation to capture emissions at the source for the grinder and bagging machine could also be an effective approach to reducing diacetyl exposure for coffee production workers to levels below the REL.

Limitations

There are a number of limitations associated with this research that could have been mitigated given a more robust budget. Exposure data for the production workers were collected for only 4 days of sampling at a single facility over a period of 1 month. The samples taken at this facility were purposefully collected during the facility's peak production season, so the results of our study represent a worst-case exposure scenario for this facility. Conducting the fieldwork at a variety of different times of the year may have given a more representative characterization of these workers' exposures to alpha-diketones. Our survey was focused on one facility which limits our ability to generalize our results across the coffee industry.

Conclusions

Results from this observational study showed that coffee production workers at this facility had elevated exposures to diacetyl and 2,3-pentanedione compared to NIOSH and ACGIH recommended exposure guidelines. Furthermore, exposure was highest on days where workers were spending more time on tasks involving ground roasted coffee (i.e. grinding and packaging ground beans) compared to days where workers were handling mainly whole roasted beans. Area emission measurements can be useful in determining what work processes are contributing to heightened exposure levels, and the results of our study showed diacetyl and 2,3-pentanedione emissions were highest at the bagging and grinding stations. Similar to previous studies, these data suggest that processing tasks associated with ground coffee are the biggest contributors to workers' exposure to diacetyl and 2,3-pentanedione. Future research could focus on designing and evaluating effective engineering controls, in the form of local exhaust ventilation, with the goal of reducing alpha-diketone emissions and exposures. Future research could also include conducting similar studies at other small-scale craft coffee roasters and cafés in order to better understand the variability in emissions and exposures across these types of facilities. Despite evidence that coffee workers are being exposed to alpha-diketones at levels above recommended guidelines, there have been few reports of increased incidence of occupational lung disease among workers in this industry. Coffee processing workers and baristas are a population with both poor surveillance data and high rates of employment turnover, so the prevalence of occupational lung disease among these workers is not known. Future research could also focus on improving exposure monitoring and medical surveillance among this population of workers, including longitudinal studies to assess the long-term health risks of exposure to naturally occurring diacetyl and other alpha-diketones (Harvey *et al.*, 2020).

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