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Optimization of roasting conditions for high-quality Arabica coffee

[1*]Ku Madihah, K.Y., [1]Zaibunnisa, A.H., [1]Norashikin, S., [1]Rozita, O. and [2]Misnawi, J.

[1]Faculty of Applied Sciences, Universiti Teknologi MARA, 40000, Shah Alam, Selangor, Malaysia
[2]Indonesian Coffee and Cocoa Research Institute, Jl.Pb.Sudirman 90, Jember 60118, Indonesia

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Abstract

Central Composite Design (CCD) was used to optimize roasting conditions (temperature and time) for Arabica coffee beans. Current method of roasting was able to give good quality beans in term of flavour but the formation of acrylamide was not studied. In this study, optimization based on high quantity of flavour compounds (pyrazines) with low level of acrylamide resulted in roasting temperature of 167ºC for 22 minutes. The coffee beans produced using the optimized conditions have the following characteristics: flavour compounds: 2,3,5 trimethyl pyrazine (0.48 mg/100 g), 2,3,5,6 tetramethyl pyrazine (0.42 mg/100 g), 2 methyl pyrazine (0.25 mg/100 g) and 2,5 dimethyl pyrazine (0.13 mg/100 g) and low concentration of acrylamide (0.11 mg/100 g) with sensory evaluation of 7.5 from 10 points. This proposed roasting condition will be very useful for coffee manufacturers in order to produce high quality coffee beans.

Introduction

Coffee is one of the most popular and widely consumed beverage mainly due to its unique flavour. Maillard reaction products (MRPs), developed during the roasting process contribute to its attractive aroma and flavour are the important factors in determining the quality of coffee. (Nicoli *et al.*, 1997). Different coffee varieties contribute to the distinctive aromatic compounds unique to each type or origin of green coffee (Bhumiratana *et al.*, 2011). Two major types of coffee beans are Arabica (*Coffea Arabica*) and Robusta (*Coffea canephora*). Arabica is more valuable because its produces better tasting beverage which is therefore more expensive than the Robusta coffee (Brohan et al., 2009).

Coffee flavor is directly related to the volatiles compounds produced during roasting as a result of a large group of complex heat-activated reactions (Agresti *et al.*, 2008). Coffee contains over 800 volatiles (Makri *et al.*, 2011) that belong to different chemical families including acids, alcohols, aldehydes, esters, furan, ketones, lactones, phenolic compounds and pyrazines. These compounds responsible for the coffee aroma and also called key odorants (Gonzales-Rios *et al.*, 2007; Brohan *et al.*, 2009; Freitas *et al.*, 1999).

Roasting is the important step in the production of coffee because it enables the development of flavour, aroma and colour. The temperature and time of roasting will influence the development of flavour compounds. Coffee aromatic compounds are formed by the reactions that occur during roasting such as Maillard reaction, Strecker degradation, degradation of sugar and breakdown of amino acids (Makri *et al.*, 2011).

Many pyrazines have been reported to contribute to roasted aromas of cooked foods, and in the case of coffee, such compounds have been associated to burnt and roasted flavours (Agresti *et al.*, 2008). Pyrazines are known to be abundant in coffee, and over 80 of such compounds have been previously detected. 2,3,5,6-tetraethylpyrazine, 2,3,5-trimethylpyrazine, 2-methylpyrazine, 2,3-dimethylpyrazine, 2,5-dimethylpyrazine and 2,6-dimethylpyrazine have been found in roasted Arabica Brazil coffees beans using SPME-headspace gas (Schiffman and Leffingwell, 1981; Sasaki *et al.*, 1986; Toci and Farah, 2008; Oliveira *et al.*, 2009; Korhonova *et al.*, 2009; Makri *et al.*, 2011).

However the formation of undesirable compounds such as acrylamide may also resulted from roasting process. Acrylamide is a well-known carcinogenic compound which is formed mostly during food processing at very high temperature such as cooking, baking, roasting, frying and sterilization due to interactions between amino acid asparagine and carbonyl source via Maillard reaction (Anese *et al.*, 2010). Acrylamide has been classified by the International Agency for Research on Cancer (IARC)

*Corresponding author.
Email: *emrik_86@yahoo.com*

as probably carcinogenic to human (IARC, 20044). Acrylamide has been detected in coffee (powder, instant and ground) ranged from 150 to 327 µg/kg (Bortolomeazzi *et al*., 2012) and about 1.16 to 2.31 µg in 30 mL of espresso Arabica coffee (Alves *et al.*, 2010). The accepted level of acrylamide in coffee products has yet been determined. According to Food and Drug Administration, the level of acrylamide in fries for consumption is 0.077 mg/kg. Even though there is no research on the effect of acrylamide on human, it has been shown to have carcinogenic effect on laboratory animal. Thus, making acrylamide as a potential carcinogenic to human.

The use of RSM in the process optimization leads to the need for an experimental design, which can generate a lot of samples for consumer evaluation in short period of time, and thus laboratory level tests are more efficient (Mendes *et al.*, 2001). Central composite design (CCD) is the most useful design for estimating multifactor response surface which keeps the numbers of experiments to a minimum while allowing simultaneous assessments of variations of all the experimented factors studied and distinguishing the interaction among them (Zaibunnisa *et al.*, 2009).

Several research have been conducted on the effect of roasting degree on formation of volatiles compounds (Maria *et al*., 1995; Hashim and Chaveron 1996; Huang *et al*., 2007; Rodrigues *et al.*, 2011) and on optimization of robusta coffee beans based on colour (Mendes *et al.*, 2001). However, there is still no research has been done on optimization of Arabica coffee beans based on pyrazines and acrylamide content. This study is focus on optimization of roasting conditions (temperature and time) of Arabica coffee bean based on pyrazines and acrylamide using Response Surface Methodology (RSM) in order to produce superior quality of roasted coffee product.

Materials and Methods

Materials

Fermented and dried Arabica coffee beans samples with moisture content of 11.26% were purchased from Andungsari plantation, Bondowoso, East Java, Indonesia.

Roasting of coffee beans

Coffee beans were roasted using a roaster (PROBAT, Germany) as suggested by Central Composite Design (CCD). Suggested temperature and time were in ranged 155 to 185^{o}C and 15 to 30 mins respectively.

Grinding and storage

Roasted coffee beans were finely ground in a coffee grinder at 3.5 screen size (0.30 mm) and keep refrigerated in sealed plastic bag prior to analysis

Analysis of acrylamide

Ground samples (5 g) were dissolved in 50 mL hot water and filtered using 0.45 mm Whatman filter paper. Solid Phase Extraction (SPE) C18 column was conditioned using 3 mL acetone and 3 mL formic acid. Filtered sample was applied to SPE tube at which the sample solution is allowed to pass through tube with gravity flow. SPE tube was washed using 2 mL distilled water and vacuum was used for 2 mins to dry the excess water. Sample was eluted using 3 mL acetone. The eluted sample was filtered using 0.45 µL syringe filter and kept at -20^{o}C until further GC-FID analysis. Analysis of acrylamide was carried out using Gas Chromatograph (Shimadzu 2010) equipped with Flame Ionization Detector with a temperature 260°C. RTX-5 column (30 m x 0.25 mm I.D. x 0.25 µm film thickness) was used with injector temperature of 260°C, helium gas at constant pressure as carrier gas, and with oven temperature of 100°C (hold 0.5 min) to 200°C at 15°C/min.

Analysis of pyrazines

Ground samples (5 g) were heated to 30°C and SPME fiber Polydimethylsyloxane-Divinyllbenzene (PDMS-DVB) was introduced to the headspace of sample for 30 mins. The fibre was reconditioned for 15 minutes into GC injection port. Flavour compounds (methyl pyrazine, dimethyl pyrazine, trimethyl pyrazine and tetramethyl pyrazine) were separated using GC-FID equipped with Rtx-5(dimethylpolisiloxane crossbone) capillary column, helium with 30 ml/min constant flow as carrier gas and injector SPL-1 operating in splitless mode. GC temperature programmed from 60^{o}C (3 min) to 180^{o}C at 5^{o}C/min for 3 min. Identification of the component of the standard was carried out by comparing the retention time of standards and quantitation using the internal standard (4-picoline) method.

Sensory evaluation

10 g samples were placed in the sensory bowl, then, water was added till full of bowl and was covered before evaluated by one expert panellist and three trained panellist from Indonesia Coffee and Cocoa Research Institutes. Sensory evaluation followed cupping system from Specialty Coffee Association of America which were based on flavour, aroma, sweetness, balance, body, acidity, aftertaste,

cleancup, uniformity and overall evaluation of the coffee bean.

Results and Discussion

Roaster (PROBAT, Germany) was used for roasting of Arabica coffee beans. The effect of two independent variables, A: temperature (150-185°C) and B: time (15-30 min) on seven response variables 2-methylpyrazine, 2,3-dimethylpyrazine, 2,5-dimethyl pyrazine, 2,3,5-trimethylpyrazine, 2,3,5,6-tetramethylpyrazine, acrylamide and overall sensory evaluation were studied by using Response Surface Methodology (RSM). For overall sensory evaluation, the characteristics used for evaluation was based on flavour, aroma, sweetness, body, uniformity, aftertaste, cleancup, balance and acidity of roasted coffee beans (Table 1). 14 treatments were assigned by using CCD. The Centre Point was repeated six times to calculate the repeatability of the method. The arrangement of CCD for independent variables and the responses is shown in Table 2. The summary of the results obtained from CCD are shown in Table 3.

The adequacy of the model was determined by using model analysis, lack of fit test and coefficient of determination (R^2). The significance of the equation parameter was assessed by F value at probability ($p > F$) less than 0.05 (Zaibunnisa *et al*., 2009).

In this study, low R^2 value was obtained for 2,3-dimethyl pyrazine 0.3656. According to (Zaibunnisa *et al*., 2009), for a good fit of a model, R^2 should be at least 0.80. This result indicates that the presence of 2,3-dimethylpyrazine in roasted coffee beans was not influenced by roasting temperature and time due to unstable characteristics of this compound. Acrylamide concentration was not influenced by roasting conditions since this compound is not stable. It will form at high temperature and also will get destroyed at certain level of extreme temperature (Gokmen *et al*., 2006).

All responses were used based on quadratic model and square root transformation. Marker compound 2-methylpyrazine, 2,5-dimethylpyrazine, 2,3,5-trimethylpyrazine, 2,3,5,6-tetramethylpyrazine and acrylamide with significant model and not significant lack of fit were used for optimisation of roasting

Table 1. Sensory evaluation of roasted Arabica coffee beans

Run	Temperature (°C)	Time (minute)	Aroma	Flavour	Aftertaste	Acidity	Body	Uniformity	Balance	Cleancup	Sweetness	Overall
1	179.90	27.80	5.69	5.25	5.38	2.00	5.88	10.00	5.25	10.00	2.50	4.75
2	167.53	22.50	7.56	7.06	7.06	6.44	7.06	10.00	7.00	10.00	10.00	7.48
3	155.15	27.80	7.06	6.44	6.19	6.06	6.63	10.00	6.38	9.25	6.75	6.38
4	167.53	22.50	7.56	7.44	7.31	7.44	7.38	10.00	7.31	10.00	10.00	7.38
5	179.90	17.20	7.69	7.63	7.31	7.00	7.44	10.00	7.38	10.00	10.00	7.50
6	155.15	17.20	6.44	6.38	6.38	6.06	5.88	10.00	6.13	10.00	10.00	6.13
7	167.53	22.50	7.25	6.63	6.63	7.31	6.56	10.00	6.75	10.00	10.00	7.50
8	167.53	30.00	7.13	6.69	6.75	6.19	6.50	10.00	6.38	10.00	10.00	6.63
9	167.53	22.50	7.13	7.38	7.44	7.06	7.31	9.50	7.56	10.00	10.00	7.50
10	150.02	22.50	7.31	7.06	7.13	7.19	7.06	10.00	6.94	10.00	10.00	7.00
11	167.53	15.00	6.38	6.69	6.94	6.81	6.50	10.00	6.44	10.00	10.00	6.69
12	185.03	22.50	6.13	5.88	5.88	3.00	6.50	10.00	5.88	10.00	5.00	5.75
13	167.53	22.50	7.50	7.56	7.31	7.50	7.50	10.00	7.56	9.50	9.50	7.56
14	167.53	22.50	7.50	7.56	7.25	7.56	7.38	9.50	7.44	10.00	10.00	7.38

Table 2. Central Composite Design arrangement for independent variables A (Temperature, °C) and B (Time, minute) and their responses; 2-Methylpyrazine, 2,3-Dimethylpyrazine, 2,5-Dimethylpyrazine, 2,3,5-Trimethylpyrazine, 2,3,5,6-Tetramethylpyrazine, acrylamide and overall sensory evaluation

Temp (°C)	Time (minute)	2-methyl Pyrazine (mg/100 g)	2,3-dimethyl Pyrazine (mg/100 g)	2,5-dimethyl pyrazine (mg/100 g)	2,3,5-trimethyl Pyrazine (mg/100 g)	2,3,5,6-tetramethyl pyrazine (mg/100 g)	Acrylamide (mg/100 g)	Overall sensory evaluation
167.53	22.50	0.22	0.45	0.12	0.58	0.37	0.13	7.48
155.15	17.20	0.10	0.15	0.09	0.08	0.31	0.16	6.13
179.90	27.80	0.05	0.05	0.08	0.02	0.07	0.25	4.75
155.15	27.80	0.15	0.76	0.13	0.07	0.13	0.80	6.38
179.90	17.20	0.03	0.44	0.14	0.09	0.11	1.75	7.50
167.53	22.50	0.29	0.54	0.11	0.60	0.39	0.12	7.38
167.53	22.50	0.24	0.36	0.15	0.14	0.49	0.11	7.50
185.03	22.50	0.05	1.15	0.07	0.25	0.16	0.68	5.75
167.53	15.00	0.10	0.39	0.09	0.07	0.19	0.53	6.69
167.53	22.50	0.24	0.46	0.13	0.57	0.39	0.11	7.50
167.53	22.50	0.25	0.40	0.12	0.55	0.35	0.10	7.56
167.53	30.00	0.05	0.04	0.10	0.04	0.07	0.89	6.63
150.02	22.50	0.03	0.04	0.03	0.03	0.05	0.30	7.00
167.53	22.50	0.23	0.43	0.45	0.45	0.53	0.10	7.38

Table 3. Summary of Central Composite Design for roasting of Arabica coffee beans

Compounds	Transform	Model	Lack of fit	R^2	Equation[a]	Significant model terms
2- Methylpyrazine	None	Quadratic Significant	Not significant	0.9114	2MP = 0.25 – 0.018A + 6.512E-004B – 0.096A2 – 0.078B2 – 6.679E-003AB	A2, B2
2,3-Dimethylpyrazine	None	2FI Not Significant	Significant	0.3656	2,3DMP = 0.41 + 0.14A – 0.033B – 0.25AB	-
2,5-Dimethylpyrazine	None	Quadratic Significant	Not significant	0.7484	2,5DMP = 0.13 + 7.334E-003A – 1.025E-003B – 0.028A2 – 6.366E-003B2 – 0.026AB	A2,AB
2,3,5-Trimethylpyrazine	None	Quadratic Significant	Not Significant	0.7803	2,3,5TMP = 0.48 + 0.036A – 0.016B – 0.18A2 – 0.22B2 – 0.018AB	A2, B2
2,3,5,6-Tetramethylpyrazine	None	Quadratic Significant	Not Significant	0.8569	2,3,5,6TP = 0.42 – 0.013A – 0.048B – 0.15A2 – 0.14B2 + 0.032AB	A2, B2
Acrylamide	None	Quadratic Significant	Significant	0.9028	Acrylamide = 0.11 + 0.20A – 0.045B + 0.22A2 + 0.33B2 – 0.54AB	A, A2
Overall sensory evaluation	None	Quadratic Significant	Significant	0.9488	Overall sensory evaluation = 7.47 – 0.13A – 0.37B – 0.50A2 – 1.11B2 – 1.00AB	B, A2, B2, AB

The central composite design was generated using Design Expert 6.0 Software
[a]A = Temperature (°C), B= Time (minute)

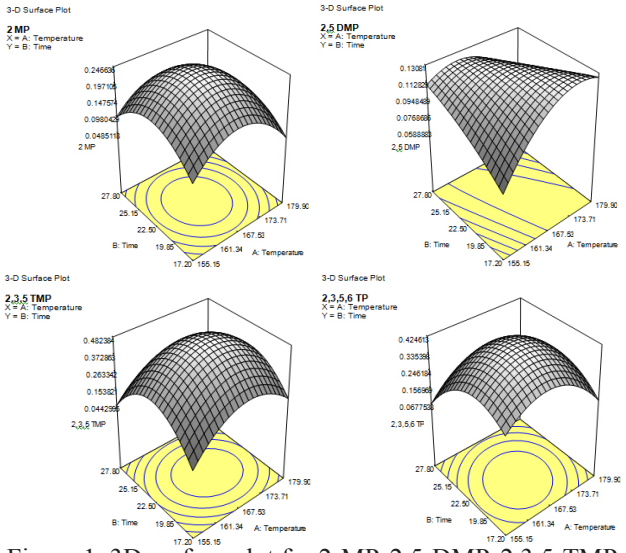

Figure 1. 3D surface plot for 2-MP, 2,5-DMP, 2,3,5-TMP and 2,3,5,6-TP from the central composite design (CCD)

condition since the presence of 2,3-dimethylpyrazine and overall sensory evaluation were not influenced by roasting temperature and time. The presence of these marker compounds significantly affect roasted coffee aroma. They were present in higher concentration in the roasted coffee aromatic oil obtained by Oliveira *et al.* (2001) using Supercritical Fluid Extraction. These compounds represent important classes of coffee aroma compounds (pyrazines).

The value of coefficient of determination (R^2) for 2-methylpyrazine, 2,5-dimethylpyrazine, 2,3,5-trimethylpyrazine and 2,3,5,6-tetramethylpyrazine were 0.9114, 0.7484, 0.7803 and 0.8569 respectively which were obtained using quadratic model. The statistical analysis of this data were significant ($p < 0.05$). The ANOVA also showed that there was a non-significant ($p > 0.05$) lack of fit which validates the model. The predicted values of all selected marker compounds were calculated using the regression model and compared with the actual value.

After producing the polynomial regression equations relating the responses to the independent variables, the optimisation procedure was performed to obtain the optimal levels of two factors (A and B). Numerical optimisation was also carried out in order to determine the optimum condition for roasting of Arabica coffee beans which give high concentration of flavour compounds and low concentration of undesirable acrylamide.

3D surface plot was constructed for all marker compounds as shown in Figure 1. Concentration of all pyrazines increased linearly in relation to the temperature and time of roasting, before starting to decrease after reached a maximum peak at 167°C for 22 mins.

The goals were set at maximum for all flavour compounds and minimum for acrylamide. The optimal condition for roasting which depends on the dependent variables was obtained using predicted equation determined by using RSM. The optimisation solution which was based on the maximum level of flavour compounds (2-methylpyrazine, 2,3-dimethylpyrazine, 2,5-dimethylpyrazine, 2,3,5-trimethyl pyrazine and 2,3,5,6-tetramethylpyrazine) and minimum level of undesirable acrylamide and obtained a temperature (A) 167.68°C and time 22.50 minute with a desirability 0.829.

Conclusion

Results obtained from this study indicates that volatile flavours compounds; 2-methylpyrazine and 2,5-dimethylpyrazine are the marker compounds that contribute to Arabica coffee flavour. Therefore, the optimized condition (time and temperature) for roasting of Arabica coffee beans is at temperature of 167.68°C for 22.50 min. Under the studied of roasting conditions, low amount of acrylamide was detected

(0.11 mg/100 g) with overall sensory evaluation of 7.5.

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