RELATIVE IMPORTANCE AND INTERACTION OF ROASTING VARIABLES IN COFFEE ROASTING PROCESS

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ABSTRACT: This work describes a study in which levels of variables that may control the coffee roasting process were set in an experimental matrix that aimed at measuring their relative importance and the interaction between variables. Each control variable was set in two levels and the combination of these levels elicited 32 different roasting procedures. The physical responses were determined for a specific roaster. Experimental planning allowed the determination of the relative influence of each control variable in each response variable for this roaster. This led to a primary quantification of the major factors that contribute to the roasting process and the relative importance of roast parameters that influence the quality of the coffee beverage. Moreover, these results indicated what interactions could occur between these parameters. The characterization of the relative influence of control variables is a first approach to model the roaster response and the coffee quality that each roasting can achieve.

Index Terms: Coffee roasting, multivariate experimental planning, coffee roasting control variables, coffee roasting response variables.

IMPORTÂNCIA RELATIVA E INTERAÇÃO DAS VARIÁVEIS DE TORRA NO PROCESSO DE TORREFAÇÃO DE CAFÉ

RESUMO: Este trabalho descreve o estudo no qual níveis de variáveis que podem controlar o processo de torrefação de café foram estabelecidos em uma matriz experimental com o objetivo de medir a importância relativa e a interação dessas variáveis. Cada variável de controle assumiu dois níveis e a combinação desses níveis resultou em 32 processos de torra diferentes. As respostas físicas foram determinadas para um torrefador específico. O planejamento experimental permitiu a determinação da influência relativa de cada variável de controle em cada variável de resposta para o torrefador estudado. Isto permitiu uma quantificação básica dos fatores que contribuíram para o processo de torrefação e a medida da importância relativa dos parâmetros de torra que influenciam a qualidade da bebida café. Além disso, estes resultados indicaram que interações podem ocorrer entre esses parâmetros. A caracterização da importância relativa das variáveis de controle é uma primeira abordagem para modelar a resposta do torrefador e a qualidade do café que pode ser alcançada em cada torra.

Termos para indexação: Torrefação de café, planejamento experimental multivariado, variáveis de controle da torra, variáveis de resposta da torra**.**

1 INTRODUCTION

Roasting description and its modelling in scientific literature

Raw coffee without roasting cannot achieve the taste and the flavor that every corner in the world knows. However, the roasting process is a complex process to control, since it involves mechanical, thermal and chemical changes that affect each other as well as the final taste and flavor of the brew. The roasting itself deeply affects the final quality of the coffee drink and the price that the final beverage can achieve (GLOESS et al., 2014; WIELAND et al., 2012; YERETZIAN et al., 2002).

The world total coffee consumption has been increasing since 2012 (ICO (1), 2016). However, the total production by all exporting countries decreased in the same period (ICO (2), 2016). The migration to better quality coffee is also a tendency detected in the USA market, despite the higher price to the final customer (VELLUCI, 2015).

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The final quality of the coffee beverage evolves from the constitution of the roasted beans, which depends on the characteristics of the raw material, as well as the post-harvest treatment conditions: processing, drying, reprocessing, storage, roasting and grinding (GIOMO, 2012).

Several steps must happen from planting to the moment that someone drinks the beverage that achieves the well-known flavor and aroma of the coffee brew that traditionally marks its quality. All post-harvest processing steps exert marked influence on the final quality of the coffee beverage, but the roasting process is the major contributor to its quality, since there is no coffee flavor without roasting. However, an improperly executed roast can mask all the characteristics preserved during the other post-harvest processing steps.

Several complex chemical reactions occur inside the coffee bean during the roasting process, leading to various physical and chemical changes in the original composition and consequent alterations in coffee flavor and aroma (MWITHIGA; JINDAL, 2003; GLOESS et al., 2014; KARYADI et al., 2009).

This process is still quite empirically controlled and the knowledge of the roaster master is one of the most important assets. Nevertheless, depictions of coffee roasting usually divide it in three stages:

The first stage (the drying phase) is the endothermic phase of the roasting, which is characterized by the drying of the green beans due to the vaporization process (GLOESS et al., 2014). Once the beans enter the roaster, the temperature of the roaster drum drops and reaches the lowest temperature achieved during roasting. The difference between the temperature of the bean inserted in the roaster and the higher temperature of the roaster itself causes the drop;

The second stage is the pyrolysis phase, when other kinds of reactions occur (GLOESS et al., 2014). In this stage, there is a major production of volatile (VOC) and semi-volatile organic compounds due to these pyrolytic reactions. The pressure increases inside the coffee bean, since gas release can occur but only when the gas is able to permeate through the bean walls. When this pressure increase overcomes the mechanical resistance of the bean walls, they crack and the beans emit a popping sound known as the first pop or first crack (YERETZIAN et al., 2002; WILSON, 2014).

The third stage is the end of the roasting process, in which the coffee beans must cool quickly (GLOESS et al., 2014; YERETZIAN et al., 2002). In this phase, the beans produce heat by themselves through exothermic reactions, and they must exit the roaster to cool immediately by exposure to ventilation or water to prevent overcooking.

Even though the roasting process occurs in stages, it can also variegate according to the quantity of beans in relation to the total volume of the roaster and to the characteristics of the product, such as species, variety and origin of the coffee. Thus, the operational conditions of roasting (time, rotation and temperature programs) are not fixed and the operator adjusts them according to the characteristics of the raw material and the quality of flavor that is attainable.

Several authors have already tried to model the roasting process, notwithstanding all its inherently complexity. Most of the works tried theoretical and semi empirical models, many of them based in the assumptions concluded by Schwartzberg and republished in 2013.

Hernandez et al. (2007) experimentally measured and modeled heat and mass transfer – moisture decrease – in coffee beans during batch roasting. Their mass transfer results deviate from the model in the exothermic step, but their modeled heat-transfer agreed very well in any isotherm below 250 ºC and the moisture model described the mass transfer with good agreement before the exothermic step. Heyd et al. (2007) tried a similar experiment but with a different mathematical approach for modelling. A thermocouple inside the coffee bean helped measure inner bean temperature. They also measured input and output air temperatures as well as bean moisture at each minute. They modeled the bean as a sphere, which could introduce sensible deviations from the measured bean behavior.

Fabbri et al. (2011) modelled heat and water loss during the roasting and compared their model to practical results. Their model was purely endothermic, and thus they reasonably modeled only the first step of roasting. Botazzi et al. (2012) numerically modelled water loss and heat transfer. They took into account more physical-chemical attributes, such as the heat produced by the beans, which increased the modelling complexity. Each attribute had its own independent differential equation without cross-linked terms and they modelled the beans as perfect spheres. They tested their models against (i) previous results of Schenker (2000) and (ii) results from an industrial coffee roaster. The authors credited the observed deviations between the modeled and measured values to the long sampling period of the data logger and to the radiation that emanates from the burner.

Putranto and Chen (2012) modeled barley and coffee roasting using another kind of modelling that started with a very simple time dependent differential equation. The determination of some thermal dependent constants was necessary for the model and they tested isothermal roastings, where each temperature generated a distinct equation. The model seemed to fit the experimental data very well for barley applications.

Romani et al. (2012) used an electronic nose (EN) and neural network (NN) computation to trace weight loss, density, moisture content, and surface color. They used the same Arabica coffee samples for different roasting times in the same roasting conditions of 200 ºC as initial temperature and with constant fuel input. They sealed each roasted sample into a glass vial for 20 hours at room temperature and the combined PCA (Principal Component Analysis) and NN analysis of the sensor responses showed a good prediction capacity.

Alonso-Torres et al. (2013) modeled heat and mass transfer in individual coffee beans with computational fluid dynamics (CFD) using a three-dimensional simulation of the bean placed in a glass tube where hot air flowed. Thousands of small geometrical domains known as mesh or grid composed the modeled bean, in which they solved differential equations using model parameters for usual roasting conditions. Higher temperatures led to some deviation from literature results, and the authors credited it to the lack of exothermic and physical expansion parameters in the model.

Chiang et al. (2017) modeled air and heat flow in a roaster oven, and took into account roaster dimensions, rotation and materials. They also modeled coffee bean heat exchange along the roasting process. They used computational fluid dynamics and numerical equations with finite volume technique. However, they modeled only the empty oven and not the effect of the bean presence. The modeled coffee bean heat exchange also ignores the exothermic contribution of the bean at the end of the roasting.

Oliveros et al. (2017) took into account porosity changes inside the bean in their coffee roasting modeling .This increased the mathematical complexity of their equations, though their model still does not incorporate bean expansion and the late exothermic step into the roasting. They compared their results with literature data and their own experiment and concluded that their premise of considering the porous void as only air was one of the reasons for model deviation from experimental data. They incorporated geometrical simulations of previous publications in their roasting modeling.

With all these limitations of model in mind, this work examined the coffee roasting process through the analysis of the roaster variables that influence the roast to build a solely empirical model and study variable importance. Multivariate experimental planning helped concoct this model and its implication can be paired with those found in previous theoretical modelling. Although this model only applies as a whole to the same conditions of this experiment, it allowed establishing correlations between roaster variables and predictions of variable effects on the roaster operation. The use of multivariate experimental planning, which generates as few experiments as possible, also helped reduce working time and experimental cost.

Experimental Planning

Experimental planning is a chemometric strategy that allows the determination of the control variables that exerts the major influence on the measured responses of a system (CALADO; MONTGOMERY, 2003; MONTGOMERY, 2013; NETO et al., 2010). This strategy helps extract more information with a lower number of experiments, which leads to time and operational cost reductions (PATIENCE, 2013).

Among the different kinds of experimental planning, the complete factorial planning is very reliable for scanning the true significance of control variables in only two setting levels. In this kind of planning, r^k usually represents the number of experiments. The number of levels is ‘r’, and ‘k’ is the number of variables. Setting levels are also usually represented by (+) and (–). This planning allows the simultaneous changing of all chosen control variables and the combination of all their setting levels. It yields not only the evaluation of control variables but can also show the occurrence of interactions between these control variables through the analysis of the measurements of response variables as well as the elimination of control variables that show no influence in responses (CALADO; MONTGOMERY, 2003; MONTGOMERY, 2013). An eventual development using three levels with the variables that showed significance can model the control/response interactions in a mathematical function.

Factorial planning (FP) helps establish correlations between control variables that alter roast response and the response variables that the operator cannot control. FP also allows establishing whether there are secondary correlations between control variables themselves. These correlations aimed at furthering the understanding of the roasting process, since the characteristic taste and aroma of coffee develop along this process. The correlation with the sensorial (or cupping) quality response of this beverage will be the subject of another work.

2 MATERIAL AND METHODS

The line of commercial roasters from Atilla Ltda. offers roasters from 2 to 60 kg. Their smallest model for 2 kg suits the trials for perfecting the roasting of specialty coffees, while it mirrors the conditions for larger roasters. This small roaster works in batches and burns gas fuel to heat both its horizontal rotating drum and the air that crosses its bean layer, while the rotation of its internal pallets permanently force the mixing of beans. Its digital controls adjust drum rotation as well as air flow speeds. Its bean cooler uses forced-air flow from top to bottom and is located in front of the drum exit to receive coffee beans at the end of the roasting time (Atilla, 2018).

Thorough discussions with the roaster manufacturers helped set the significant control variables and their meaningful ranges as well as the levels to measure within these ranges. Moreover, the discussion elicited what should be the sensible response variables that would support the aim of verifying the relationship with control variables and an attainable coffee quality.

The results obtained using complete factorial planning helped establish correlations between the control variables that may determine the roasting profile and affect coffee quality and the response/operational variables that may vary with roasting conditions. The roast manufacturing company helped in all procedures. Table 1 shows control variables and their levels.

The factorial design combination of five variables at two levels elicited 32 (2^5) combinations or 32 different roasting conditions that followed the experimental matrix (Table 2).

These numbers of variables and levels – even though they do not allow the full modelling of the relation between control and response variables – determine a mathematical model in which the coefficients show the relative importance of each variable and of each interaction of two or more variables (Equation 1). Response variable results allow the calculation of these coefficients.

$$Y = b_0 + b_1x_1 + b_2x_2 + b_3x_3 + b_4x_4 + b_5x_5 + b_{12}x_1x_2 + b_{13}x_1x_3 + b_{14}x_1x_4 + b_{15}x_1x_5 + b_{23}x_2x_3 + b_{24}x_2x_4 + b_{25}x_2x_5 + b_{34}x_3x_4 + b_{35}x_3x_5 + b_{45}x_4x_5 + b_{123}x_1x_2x_3 + b_{124}x_1x_2x_4 + b_{125}x_1x_2x_5 + b_{134}x_1x_3x_4 + b_{135}x_1x_3x_5 + b_{145}x_1x_4x_5 + b_{234}x_2x_3x_4 + b_{235}x_2x_3x_5 + b_{245}x_2x_4x_5 + b_{345}x_3x_4x_5 + b_{1234}x_1x_2x_3x_4 + b_{1235}x_1x_2x_3x_5 + b_{1245}x_1x_2x_4x_5 + b_{1345}x_1x_3x_4x_5 + b_{2345}x_2x_3x_4x_5 + b_{12345}x_1x_2x_3x_4x_5$$

However, other six roastings aside the roasting conditions of the experimental matrix in Table 2 allowed the evaluation of experimental error and robustness. These control roastings occurred at the beginning, in the middle and at the end of each workday. Their conditions (Table 3) were different from any set of conditions employed in the experimental matrix.

The 2 kg Atilla Gold Plus roaster performed all 38 roastings in two days. Each roasting used 500 g of the same homogeneous coffee with all beans above 16 sieve. A coffee producer – Sitio Bela Vista – naturally processed (without peeling off coffee fruit) coffee beans in an open drier. This producer cultivated this coffee in high altitude – 1100 m – and kindly selected and provided the Arabica coffee of variety red catucaí 785 (Catucaí Vermelho 785) that he harvested in the previous harvest season.

It is worth to emphasize that bean sieving is a common procedure that helps (i) classify that parcel of coffee in relation to the size distribution of the beans and (ii) obtain a more homogeneous and uniform roast containing beans of roughly the same size. High size beans (larger than sieve 16) usually come from higher altitudes and have better cupping performance. The correlation between size and quality is not mandatory, since there are other factors that can affect coffee quality before roasting, but larger and homogeneous sizes are preferred (ICO (3), 2016).

Mathematical calculations in Excel established the correlation between control variables – and their levels – (Table 1 and Table 5) with operational/physical variables, which are mass reduction (%), minimum temperature along the roasting (°C), cracking temperature (°C), cracking time (min:sec), and final temperature (°C).

TABLE 1 - Control variables and their chosen levels.

Control variables	Superior Level (+)	Inferior Level (-)
Roaster starting temperature (x_1)	160 °C	200 °C
Vent opening (x_2)	25-50-100 (%)	25-75-100 (%)
Rotation speed (x_3)	40-65 rpm	65 rpm
Time after the first cracking (x_4)	1 min	2 min
Fuel flow increase (x_5)	0.5 L min^{-1}	1 L min^{-1}

TABLE 2 - Experimental Matrix.

Experiment	T_0 (°C) $\mathbf{X_1}$	Vent (%) $\mathbf{X_2}$	Rotation speed (rpm) $\mathbf{X_3}$	Fuel flow increase (mbar/min) $\mathbf{X_4}$	Time after cracking (min) $\mathbf{X_5}$
1	160	25-50-100	40-65	0,5	1
2	200	25-50-100	40-65	0,5	1
3	160	25-75-100	40-65	0,5	1
4	200	25-75-100	40-65	0,5	1
5	160	25-50-100	65	0,5	1
6	200	25-50-100	65	0,5	1
7	160	25-75-100	65	0,5	1
8	200	25-75-100	65	0,5	1
9	160	25-50-100	40-65	1	1
10	200	25-50-100	40-65	1	1
11	160	25-75-100	40-65	1	1
12	200	25-75-100	40-65	1	1
13	160	25-50-100	65	1	1
14	200	25-50-100	65	1	1
15	160	25-75-100	65	1	1
16	200	25-75-100	65	1	1
17	160	25-50-100	40-65	0,5	2
18	200	25-50-100	40-65	0,5	2
19	160	25-75-100	40-65	0,5	2
20	200	25-75-100	40-65	0,5	2
21	160	25-50-100	65	0,5	2
22	200	25-50-100	65	0,5	2
23	160	25-75-100	65	0,5	2
24	200	25-75-100	65	0,5	2
25	160	25-50-100	40-65	1	2
26	200	25-50-100	40-65	1	2
27	160	25-75-100	40-65	1	2
28	200	25-75-100	40-65	1	2
29	160	25-50-100	65	1	2
30	200	25-50-100	65	1	2
31	160	25-75-100	65	1	2
32	200	25-75-100	65	1	2

TABLE 3 - Control Roasting Conditions.

Parameters	Conditions				
Starting temperature	185 °C				
Vent opening	100%				
Rotation speed	65 rpm				
Air flow	**Initial**			**From 6,5 min on**	
	1740			1800	
Pressure (Fuel flow)	**0.00 – 4.00 min**	**4.50 – 7.00 min**	**7.50 – 9.00 min**	**9.50 -10.50 min**	**11.00 min - end**
	3.5 mbar	4.5 mbar	8.0 mbar	9.5 mbar	0.5 mbar

The measurement of the above-mentioned operational variables during the roasting helped evaluate how the operational – or response – variables changed with alterations in control variables. Thermocouples type k located inside the roaster's drum in two positions allowed the measurements of oven temperature and coffee bean temperature during roasting. The mass reduction was measured by weighing the coffee beans before and after the roast in room temperature and using a scale (Urano UDC 15/5 POP). The hearing of the cracking sound determined the cracking time and the chronometer of a cell phone Samsung measured the cracking time.

3 RESULTS AND DISCUSSIONS

During each roast, the temperature was recorded every half minute and the roasting/temperature profiles were established as a function of time (Figure 1).

Confidence Intervals for roasting profiles

Control roastings apart from the roasting set of experiments and developed by the roast master helped determine the error for each experiment and the robustness of the equipment. The roast master performed this kind of roast in the same way and following the same parameters a few times throughout the two days of work (Table 3). In total, six control roastings were performed (three on the first and three on the second day). Based on these roasts, the standard deviations and confidence intervals (CI) were calculated (i) for the roast profiles obtained during the experiment and (ii) for the results obtained for the response variables.

Confidence intervals calculated from these data, represented the deviation of each control roasting from the average roast (Table 4). Figure 1 shows that the variation between control roastings is small when compared to all roastings. Thus, although there were significant variations in room temperature between control roastings, the stability of the measurements showed that the roaster was robust and only small variations between profiles occurred.

Confidence Intervals for roasting control variables

The coefficients calculated using the model of equation 1 allowed the determination of the relative influence of control variables upon each operational variable. The interaction coefficients of three or more control variables on each operational variable allowed the calculation of confidence intervals (CI) for each response function and the elimination of coefficients that were inside the confidence interval, since these interactions are consistently considered as errors (MYERS et al., 2016; NATRELLA, 2005; NETO et al., 2010; BOX et al., 2005). Table 5 exhibits the retained coefficients that remained after the evaluation of confidence intervals.

The analysis of results showed that 'time after cracking' exerts the largest and positive influence on mass reduction, that is, the increment of its time increases the mass loss. On the other hand, 'vent' exerts a negative influence on mass loss that decreases when it increases, possibly because of temperature reduction.

The initial roasting temperature (T_o) has a major and positive influence on the lowest temperature along roasting. Thus, the higher the initial temperature, the higher the lowest temperature along roasting. The rotation exerts a negative influence on the lowest temperature, so that the increase of rotation lowers the lowest temperature of the roasting process.

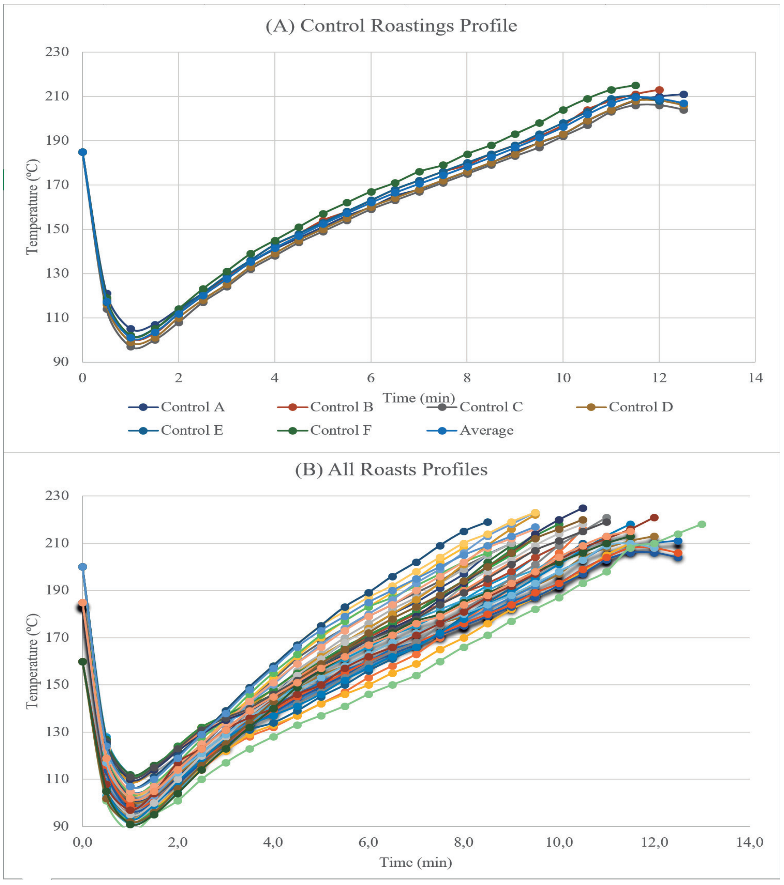

FIGURE 1 - (A) Roast profiles of control roastings and the average roasting. (B) Profiles of all roasts executed in the experimental planning.

TABLE 4 - Confidence intervals obtained from control roasting profiles.

	Control A	Control B	Control C	Control D	Control E	Control F
Standard deviation	0,47	0,28	0,71	0,45	0,27	1,06
n	26	25	26	26	25	24
t (n,α)	2,056	2,060	2,056	2,056	2,060	2,064
CI	0,19	0,12	0,29	0,18	0,11	0,45

TABLE 5 - Control variables and one interaction versus operational/response variables.

	T_0	Vent	Rotation	Fuel increase	Time after cracking	T_0 × Rotation	CI*
Mass reduction		-0.56			1.56		0.385
Lowest temperature	14.12		-3.12			-2.5	1.514
Cracking temperature				-1.19			0.804
Cracking time	-1.35	0.53	-1.11				0.241
Final temperature		-2.75	-2	2	10.12		1.652

*Following the model of BOX et al., 2005. See supplementary material for calculation details.

The interaction between T_o and rotation exerts a negative influence on the lowest temperature. The fuel flow increase is the only variable that exerts negative influence in cracking temperature, e.g. if the fuel flow increases, the cracking temperature lowers.

Three variables exert influence on the time after cracking or cracking time. Initial temperature (T_o) has the highest but negative influence: it dwindles the cracking time when it rises. The rotation also exerts a negative influence on cracking time, so that the use of the higher rotation all the time dwindles the cracking time. The only minor positive influence is vent overture that increases the cracking time when the rise in vent overture is steeper.

The roasting time after cracking exerts the most positive influence on final temperature, although fuel flow also show a positive influence on this variable. Vent and rotation exert negative influence on this variable in this order of importance.

The results obtained evaluating the control roastings to each response variable as a function of the alterations in control variables helped determine the confidence interval (CI) of response variables. The coefficient of variation (CV) establishes a better comparison between measurements, since it is a percentage, which allows the comparison of dispersions even though they result of different measurements and have different units and ranges. Table 6 presents these results for CI and CV. The CV range was from 0.74 to 5.21 %, which is a low range for this kind of measurement.

4 CONCLUSIONS

Our study elucidated the positive and negative influence of control variables and the occurrence of correlations between them. This led to a primary quantification of the major factors that contribute to the roasting process and eventually to the quality of the coffee beverage. Even though these results showed the common knowledge among roast masters and professionals in the area, they also provided an in-depth knowledge about the roaster operation, since it was possible to quantify the relative importance of roast parameters. Besides, these results indicated the interaction between parameters.

The study of response variables elicited some specific conclusions:

*the initial temperature exerts a strong influence in the lowest oven temperature;

*vent and rotation alone do not show a strong influence in any response variable;

*only the increase of fuel speed influences the cracking temperature;

*the time after cracking exerts the largest influence on mass reduction and final temperature; and

*the interaction between initial temperature and rotation influences the lowest oven temperature.

The analysis of control roasts showed that the equipment used is robust regardless external variations of temperature and humidity. The control roasts were similar to each other in the roasting profiles and in the results obtained for the response variables.

TABLE 6 - Confidence intervals for response variables in control roastings.

Controls	Mass Reduction (%)	Lowest Temperature (°C)	Cracking Temperature (°C)	Cracking Time (min)	Final Temperature (°C)
A	17	105	202	10,75	211
B	16	101	200	10,32	208
C	15	97	203	11,00	204
D	16	99	204	11,00	205
E	15	102	204	10,55	205
F	15	102	203	9,90	215
Average	15,67	101,00	202,67	10,59	208,00
Standard Deviation	0,82	2,76	1,51	0,43	4,29
CI	0,86	2,89	1,58	0,45	4,50
CV (%)	5,21	2,73	0,74	4,04	2,06

Our study highlighted the importance and influence of a set of main variables upon the roasting process and as far as we are concerned this is the first approach to this process using multivariate planning tools.

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