



## EMPIRICAL MODEL OF THE CHLOROGENIC ACID DEGRADATION KINETICS DURING COFFEE ROASTING IN A SPOUTED BED

### MODELO EMPÍRICO DE LA CINÉTICA DE DEGRADACIÓN DE ÁCIDO CLOROGENICO DURANTE EL TOSTADO DE CAFÉ EN UN LECHO FUENTE

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#### Abstract

Chlorogenic acid (5-O-caffeoylquinic acid or 5-CQA) is a biological active compound found at high concentrations in green coffee that degrades during the roasting process. In the present study coffee was roasted at three air temperatures (425, 450 and 475°C) and seven different times in an innovative spouted bed system. Bean temperature was measured at the exit of the system and 5-CQA was quantified by HPLC. In order to describe the changes in concentration during the roasting process, as a function of bean temperature, an Arrhenius type kinetic model was proposed. Bean temperature was fitted to a one linear and two exponential terms equation, as a function of time and air temperature. The parameters of the kinetic model were found by a Nelder-Mead optimization technique, and were used to propose linear equations that described them as function of air temperature. The kinetic model showed good agreement with experimental data, especially at higher temperatures ( $R^2 > 0.995$ , RMSECV  $< 4\%$ ).

**Keywords:** chlorogenic acid, spouted bed, kinetic model, optimization, coffee roasting.

#### Resumen

El ácido clorogénico (ácido 5-O-cafeoilquínico o 5-CQA) es un compuesto con actividad biológica que se encuentra presente en cantidades importantes en el café verde y cuya concentración disminuye durante el tostado. En este trabajo se utilizó un innovador sistema de lecho fuente para tostar café a tres diferentes temperaturas de aire (425, 450 y 475°C) y siete diferentes tiempos. Se monitoreó la temperatura del grano a la salida y se cuantificó el 5-CQA por HPLC. Se propuso una ecuación del tipo de Arrhenius como modelo cinético para describir los cambios de concentración durante el proceso de tostado en función de la temperatura del grano. La temperatura del grano se expresó en función del tiempo y la temperatura del aire con una ecuación con un término lineal y dos términos exponenciales. Los parámetros del modelo cinético se obtuvieron mediante un algoritmo de optimización de Nelder-Mead y a partir de ellos se propusieron ecuaciones lineales para los parámetros en función de la temperatura del aire. El modelo cinético presentó un buen ajuste a los datos experimentales, especialmente a las temperaturas más elevadas ( $R^2 > 0.995$ , CVRMSE  $< 4\%$ ).

**Palabras clave:** ácido clorogénico, lecho fuente, modelo cinético, optimización, tostado de café.

## 1 Introduction

Roasting is a key thermal process on the production of quality coffee. It changes the chemical, physical, structural and sensory properties of green coffee beans (Fabbri *et al.*, 2011). The degradation of chlorogenic acids is one of the substantial chemical changes in roasted coffee. Chlorogenic acids are

the most important phenolic compounds in coffee, accounting for 6 to 10% of green coffee. The main isomer subgroups of chlorogenic acids are caffeoylquinic, feruloylquinic and dicaffeoylquinic acids. Amongst them, 5-O-caffeoylquinic acid (5-CQA) is the most abundant isomer in coffee, and it is usually referred to as *chlorogenic acid* (Clifford, 1999; Farah, 2012; Farah & Donangelo, 2006). It has been demonstrated that chlorogenic acids

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exhibit diverse biologic activities, such as antioxidant and anti-inflammatory, as well as antihypertensive, hypoglycemic and hypolipidemic effects (Bassoli *et al.*, 2008; Wan *et al.*, 2013; Watanabe *et al.*, 2006; Yun *et al.*, 2012; Zhao *et al.*, 2012). The fate of all chlorogenic acids during roasting is still unknown. However, it is recognized that they are involved in dehydration, isomerization, epimerization, hydrolysis and polymerization reactions (Clifford, 2000; Farah, 2012). Depending on the roasting degree, the chlorogenic acid content can be reduced up to less than 1% of the original content (Farah, 2012).

In order to accomplish the roasting process, coffee beans are heated by conduction, radiation or convection (Eggers & Pietsch, 2001), and the proper -necessary- movement of the beans is achieved by rotation or by the flow of hot gases (Fabbri *et al.*, 2011). The most commonly used equipment in the industry are rotary drums, in which the beans are mixed with hot gases in a horizontal rotary drum, or in a vertical drum with paddles, and where the heat transfer is mainly by conduction. Another kind of equipment are the fluid bed and spouted bed roasters; these use high-velocity gas flows to move and heat the beans in the roasting chamber, which leads to a better heat transfer, that is mainly achieved by convection (Baggenstoss *et al.*, 2008; Eggers & Pietsch, 2001).

In general, coffee roasting conditions have an important impact on the physical and chemical changes that happen during the process. Of particular interest are the applied time-temperature profiles, which depend on the heat transfer mechanism used in the system, the temperature and the process time (Baggenstoss *et al.*, 2008; Schenker, 2000). According to Moon and Shibamoto (2010), the total concentration of chlorogenic acids is reduced as the roasting conditions intensity increases: the total chlorogenic acids content when roasting at 230°C and 12 minutes is reduced approximately by 50%, while at 250°C and 21 minutes the content is reduced to trace levels. Budryn *et al.* (2014) reported that the 5-CQA losses were higher as the roasting temperature and the air moisture increased. Perrone *et al.* (2010) studied the chlorogenic acids degradation at different times and temperatures in a commercial spouted bed roaster, finding a higher decrease of the compounds at higher process temperatures. They also evaluated an Arrhenius -first order- model to describe the changes in the total content of chlorogenic acids (9 isomers). In this model the degradation is described as a function of air temperature, so the process is considered isothermal.

In the present work, roasting was carried out in

an innovative spouted bed (MX/a/2016/016495, 2016; PCT/MX 2017/000147, 2017) that has a characteristic geometry and which, as a result of its configuration, does not have dead zones nor mobile parts; it has a draft tube that allows roasting with low pressure drops. For this specific design, the evaluation and modeling of moisture and color changes during coffee roasting has been reported (Virgen-Navarro *et al.*, 2016a; Virgen-Navarro *et al.*, 2016b), as well as the concentration changes of polycyclic aromatic hydrocarbons (Guatemala-Morales *et al.*, 2016); however, the chlorogenic acid degradation has not been studied in this roaster. Therefore the aim of this work was to study the chlorogenic acid degradation (5-CQA) during coffee roasting in this spouted bed, and to obtain an empirical model that describes the degradation kinetics as function of the process conditions (time and air temperature). The process was considered to be non-isothermal since the bean temperature changes during the process.

## 2 Materials and methods

### 2.1 Coffee roasting

Green coffee beans (*Coffea arabica*) from Talpa de Allende, Jalisco, Mexico, were roasted in the spouted bed of Fig. 1. This system comprises two regions: annulus and draft tube. Solids are fed from the top, filling the annulus region. The particles that accumulate at the bottom of the draft tube rise through it as a result of the compressed hot air stream that enters the system through a nozzle situated at the bottom left corner, generating the characteristic spout in the top and promoting the cyclic movement of particles. Once the roasting time is over, solids are discharged on the bottom (MX/a/2016/016495, 2016; PCT/MX 2017/000147, 2017). The air temperature is measured right before it enters the bed.

Batches of 1.5 kg were roasted, with an air pressure of 2 kg<sub>f</sub>/cm<sup>2</sup> and a 120 L/min flow, at seven different times and three air temperatures, as shown in Table 1. The experimental points were chosen according to preliminary runs and aiming to have the same amount of points per temperature and to achieve a similar roasting degree. Roasting was performed by duplicate.

When the roasting time was over, the whole coffee batch was discharged and the bean temperature was measured -right at the outlet- with and infrared thermometer (4470, Traceable, US).

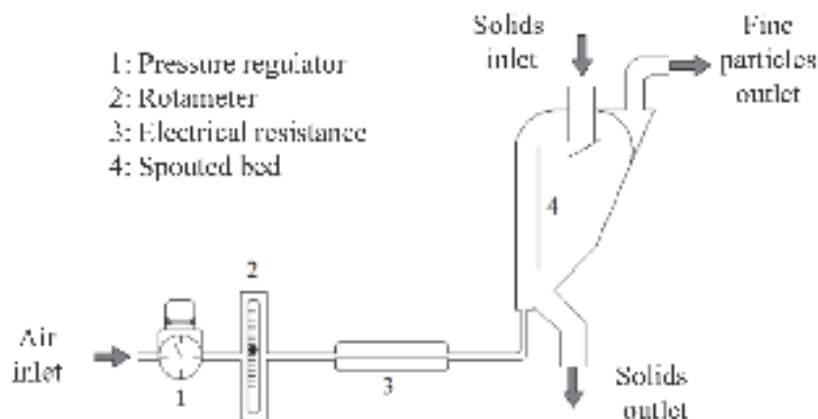


Fig. 1. Spouted bed scheme.

Table 1. Roasting conditions.

Air temperature ( $T_a$ , °C)	425	450	475
Time (t, min)	6	5.25	4.5
	12	10.5	9
	18	15.75	13.5
	24	21	18
	30	26.25	22.5
	36	31.5	27
	42	36.75	31.5

Immediately afterwards, the beans were cooled by forced convection, placing them in a metallic tray against a fan and stirring them manually until they reached room temperature, in order to stop the chemical reactions. The moisture content was determined based on the Mexican regulation NMX-F-013-2000, so coffee beans were grinded in a disc mill (Maren 1.5HP, Pulvex, Mexico) and the pulverized coffee was sieved for 5 minutes to attain a particle size smaller than 0.595 mm. Moisture content data were used to calculate the chlorogenic acid content in dry basis. Finally, the grinded and sieved coffee samples were vacuum-packed and stored at  $-10^{\circ}\text{C}$  for the further extraction of chlorogenic acid.

## 2.2 Chlorogenic acid quantification

Chlorogenic acid extraction from green and roasted samples was done according to the method reported by Meinhart *et al.* (2017). 0.5 g of grinded coffee were extracted with 14.6 mL of a 32.4% aqueous ethanol solution (HPLC grade, JTBaker, US) in a 100 mL volumetric flask. The extraction conditions

were  $60^{\circ}\text{C}$  and 250 rpm magnetic stirring (C-Mag HS4, IKA, Germany). Once the extraction time was over, the volume was made up to 100 mL with the same extraction solution. Solids were removed with filter paper (No.1, Whatman, US). Extraction was carried out by duplicate and the extracts were stored in amber glass containers under refrigeration ( $8^{\circ}\text{C}$ , REB634, Nieto, Mexico) to prevent the evaporation of the solution solvent until quantification.

Quantification of chlorogenic acid (5-CQA) was done by high performance liquid chromatography (HPLC) based on the method reported Fujioka and Shibamoto (2008). A Waters chromatograph was used, with a C-18 reversed phase column (Kromasil, 250 x 4.6 mm, 5  $\mu\text{m}$ , Akzo Nobel, US). Samples were cleaned up with a C-18 cartridge (Sep-pak, Waters, US) and a 0.45  $\mu\text{m}$  syringe filter (Millipore, U.S.A) before their injection. The injection volume was 20  $\mu\text{l}$  and each sample was injected by duplicate. The mobile phase was phosphoric acid 5mM (Karal, Mexico) and methanol (Sigma-Aldrich, US), and was injected with the following elution gradient: 85/15 from 0 to 5 min, 80/20 from 6 to 10 min, 60/40 from 11 to 20 min, 70/30 from 21 to 25 min, 80/20 from 26 to 30 min y 85/15 from 31 to 35 min. The mobile phase flow was 1 mL/min and the analysis was carried out at room temperature. A diode array detector was used (996, Waters, US), selecting a wavelength of 325 nm to measure the absorbance of 5-CQA. For the calibration curve, standard solutions of 5-CQA (USP Standard, Sigma-Aldrich, US) were prepared in methanol, with the following concentrations: 400, 300, 200, 100, 80, 40 and 10  $\mu\text{g/mL}$ .

### 2.3 Kinetic model

The most general way to describe the degradation kinetics of a compound is presented in Eq. (1), where  $C$  is the compound concentration,  $t$  is time,  $k$  is the reaction velocity constant and  $n$  is the reaction order.

$$-\frac{dC}{dt} = kC^n \quad (1)$$

Reaction velocity is usually dependent on temperature, and the Arrhenius equation is widely used to describe it (Félix-Navarro et al., 2017; Solís-García et al., 2017). In this work it is proposed that the reaction velocity dependence on temperature follows an Arrhenius type equation, as shown in Eq. (2) (van Boekel, 2009).

$$k = Ae^{(B/T)} \quad (2)$$

For coffee roasting in the spouted bed it has been observed that the temperature at which reactions really occurs is the bean temperature ( $T_p$ ); this temperature is not constant during the process and it differs from air temperature (even though it depends on it). Therefore, the kinetic -empirical- model to evaluate in this work is the one presented in Eq. (3). Parameters  $A$ ,  $B$  and  $n$  are fitting parameters without physical meaning (van Boekel, 2009); they can be regarded as pseudo parameters (preexponential factor, activation energy and reaction order, respectively) (Reyes-Valadez et al., 2016). This is because distinctly from the models that use the original Arrhenius equation, a single reaction of chlorogenic acid is not under study; chlorogenic acid content decrease is attributed to complex reaction mechanisms. Bean temperature ( $T_p$ ) is expressed as function of time ( $t$ ) and air temperature ( $T_a$ ).

$$\frac{dC}{dt} = -Ae^{\left(\frac{B}{T_p(t,T_a)}\right)}C^n \quad (3)$$

The first step was to find an empirical expression that relates bean temperature with the operation conditions: time and air temperature. For that reason, polynomial and exponential fits of the experimental data were evaluated using the *CurveFitting* toolbox of the software MATLAB®.

Once an expression for particle temperature was found, an optimization algorithm of the  $A$ ,  $B$  and  $n$  parameters of the kinetic model was developed. A simplex Nelder-Mead algorithm (*fminsearch* in MATLAB®) was used to find the optimum  $A$ ,  $B$  and  $n$  for each air temperature. This algorithm has been widely used to solve parameter optimization problems

since it minimizes a non-linear function of multiple variables. It makes optimization without restrictions, is robust to the local minima of the function, it is easy to implement and has a reasonable convergence speed (Barati, 2011; Dochain, 2008; Nelder & Mead, 1965). The objective function to minimize was the root square mean error (RMSE) between the predicted and experimental values. The predicted values by the model were found by numerical integration of Eq. (3) using the fourth and fifth order Runge-Kutta method (*ode45* in MATLAB®). The initial value of the parameters in the optimization algorithm for the three air temperatures were  $A = 10 \text{ min}^{-1}$ ,  $B = -1000^\circ\text{C}$  and  $n = 1(-)$ . In order to get a unique and generalized model for all temperatures, in the range of  $425^\circ\text{C}$  to  $475^\circ\text{C}$ , a linear relationship with respect to air temperature for the model parameters was used.

Finally, the kinetic model -proposed in this work- was compared to a similar model in which the reaction temperature is considered to be constant and to be the air temperature, as shown in Eq. (4).

$$\frac{dC}{dt} = -Ae^{\left(\frac{B}{T_a}\right)}C^n \quad (4)$$

The goodness of fit of the models was assessed using the root mean square error (RMSE), the coefficient of variation of the square root mean error (RMSECV%) and the determination coefficient ( $R^2$ ). The coefficient of variation of the RMSE is defined as the percentage RMSE with respect to the mean of the data.

## 3 Results and discussion

### 3.1 Coffee roasting

As stated previously, coffee was roasted at three air temperatures in the spouted bed; the results of particle temperature, moisture content and 5-CQA content for each evaluated time are shown in Table 2. It can be appreciated that, depending on air temperature, bean temperature changes markedly during the process, which validates the relevance of the proposed model that takes them into account. Final bean temperature has been related to roasting degree, so a similar final roasting degree was achieved with the three treatments; according to Davids (2003) these temperatures would correspond to a medium or medium dark roast.

Table 2. Particle temperature, moisture and 5-CQA content in roasted coffee at different conditions.

$T_a = 425\text{ }^\circ\text{C}$				$T_a = 450\text{ }^\circ\text{C}$				$T_a = 475\text{ }^\circ\text{C}$			
t (min)	$T_p$ ( $^\circ\text{C}$ )	%H	C (mg/g dry)	t (min)	$T_p$ ( $^\circ\text{C}$ )	%H	C (mg/g dry)	t (min)	$T_p$ ( $^\circ\text{C}$ )	%H	C (mg/g dry)
0	25	8.14±0.47	29.58±1.76	0	25	8.14±0.47	29.58±1.76	0	25	8.14±0.47	29.58±1.76
6	121.9±2.9	6.36±0.67	27.19±0.98	5.25	125.9±2.2	6.14±0.16	28.45±0.72	4.5	140.3±2.3	6.32±1.07	28.71±0.34
12	159.1±7.6	4.57±0.48	27.26±2.12	10.5	156.6±11.7	4.64±0.71	26.85±1.41	9	160.3±9.6	4.76±0.90	27.45±0.22
18	166.5±3.8	3.93±0.20	24.09±0.44	15.75	170.1±8.3	3.59±0.63	23.83±2.26	13.5	169.9±2.6	3.91±0.17	24.33±0.73
24	183.4±7.0	1.94±0.67	17.81±1.89	21	193.9±3.4	2.63±0.41	15.98±1.83	18	189.3±2.6	2.86±0.30	18.01±0.59
30	201.5±6.4	1.91±0.61	10.31±3.53	26.25	198.8±3.1	1.90±0.78	11.43±2.47	22.5	197.1±4.2	2.69±0.47	14.04±1.19
36	209.5±0.7	1.22±0.24	5.79±0.08	31.5	212.0±1.4	1.07±0.18	6.47±1.71	27	216.0±17.0	1.39±0.12	8.31±0.76
42	219±22.6	1.49±0.15	5.40±4.74	36.75	225±12.7	1.36±0.35	2.53±2.31	31.5	222±4.2	1.59±0.32	3.28±0.58

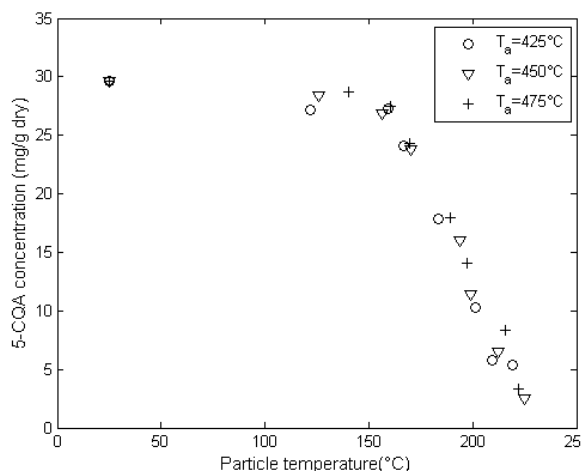


Fig. 2. Effect of particle temperature on 5-CQA content.

For moisture content, the percentage was calculated as g water/g wet coffee; initial and final values (8 and 1.5%) are very similar to the reported for coffee roasting in a conventional spouted bed roaster (Heyd *et al.*, 2007). This moisture data were used to calculate 5-CQA content on dry basis.

The content of 5-CQA found in green beans, of 29.58 mg/g dry, is within the expected range for *Coffea arabica*, where concentrations of 10-55 mg/g dry have been found (Farah *et al.*, 2005; Kitzberger *et al.*, 2014; Marín & Puerta, 2008; Moon & Shibamoto, 2009; Tfouni *et al.*, 2012). On the other hand, the concentrations found in the final roasted product of 2.53 to 5.40 mg/g dry, are also similar to the previously reported for medium or medium dark roasted coffee (2-6 mg/g dry) (Farah *et al.*, 2005; Fujioka & Shibamoto, 2008; Tfouni *et al.*, 2012).

When looking at the 5-CQA content changes with respect to bean temperature, an important change above 170°C is observed. This behavior is shown in Fig. 2: at temperatures above 150°C the decrease in 5-CQA content starts to speed up, especially between

150 and 170°C. This behavior was the same at all air temperatures, which, once more, confirms the pertinence of expressing the degradation kinetics of 5-CQA as a function of particle temperature, and not only as function of the process air temperature.

### 3.2 Particle temperature model, $T_p$

Polynomial and exponential expressions were evaluated using the *CurveFitting* toolbox of MATLAB® in order to find a proper model for particle temperature as a function of time and air temperature. When considering both factors, the best fits were found with polynomial expressions (third order for one of the variables), but still the RMSE value was high, lacking a good fit. Hence, afterwards, only the time variable was considered, finding one equation for each temperature. This procedure allowed for better fits with two exponential term expressions. Therefore, with the aim of having a single expression for all the temperature range of the process, and as a function of both factors (time and air temperature), the model in Eq. (5) was considered. This model takes into account two exponential terms for the time, but it also includes a fitting linear term using air temperature.

$$T_p = (p_0 T_a) + (p_1 e^{qt}) + (p_2 e^{st}) \quad (5)$$

Parameters of Eq. (5) were found ( $p_0 = 0.2914$  (-),  $p_1 = -136.4$  (-),  $p_2 = -31.05$  (-),  $q = -0.2317\text{ min}^{-1}$ ,  $s = 0.029\text{ min}^{-1}$ ), as well the goodness of fit values.  $R^2$  was 0.990, RMSE was 6.791, and RMSECV was 4.16%, so it was considered a good fit. The fit of the experimental data to the model for each temperature is shown in Fig. 3.

As it can be noted, the model follows the trend of the experimental data, and the behavior of the particle temperature is similar to the reported by other authors; at the earlier times of the process temperature increases rapidly, while it increases at a lower rate at latter stages (Fabbri *et al.*, 2011; Heyd *et al.*, 2007).



Table 3. Obtained parameters and kinetic model fit.

Parameter	A (min <sup>-1</sup> )	B (°C)	n (-)	R <sup>2</sup>	RMSE	RMSECV (%)
Equation	$A = -0.2256T_a + 127.76$	$B = 12.175T_a - 6532.5$	$n = -0.0204T_a + 10.071$			
$T_a = 425\text{ °C}$	31.8758**	-1358.063**	1.3852**	0.978	1.407	7.6
$T_a = 450\text{ °C}$	26.2346*	-1053.6833*	0.8743*	0.995	0.672	3.7
$T_a = 475\text{ °C}$	20.5943*	-749.3036*	0.3634*	0.998	0.479	2.5

\*Obtained initially with the parameter optimization algorithm

\*\*Obtained with the linear equation

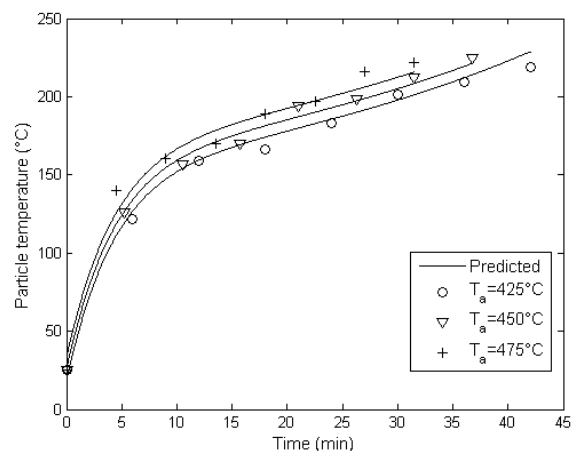
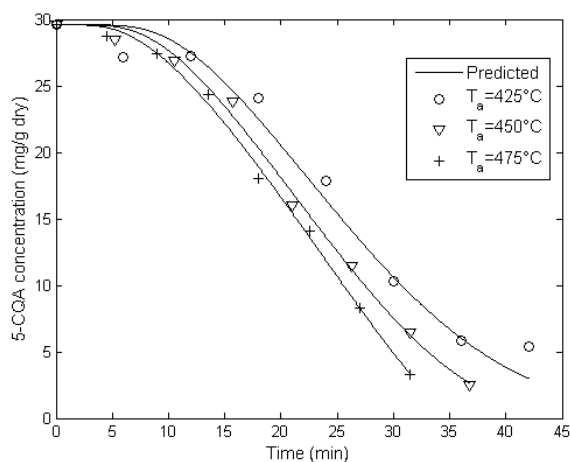


Fig. 3. Effect of air temperature and time on particle temperature.

### 3.3 Kinetic model

The particle temperature model was used to implement the parameter optimization algorithm of the kinetic model of Eq. (3). The initial values were:  $A = 10\text{ min}^{-1}$ ,  $B = -1000\text{ °C}$  and  $n = 1$  (-). The obtained parameters with the optimization algorithm for 450°C and 475°C are presented in Table 3. The fit to the kinetic model to the 5-CQA degradation with the obtained parameters is good ( $R^2 > 0.990$  and  $\text{RMSECV} < 4\%$ ), and the parameters follow a trend ( $A$  and  $n$  decrease with temperature, and  $B$  increases). For the temperature of 425°C, the fit with the optimized parameters has an  $R^2$  of 0.984 and a  $\text{RMSECV}$  of 6.5%, but the values of the parameters did not show a relationship with the ones obtained at 450°C and 475°C; this might be due to two experimental values (at 6 and 42 minutes) at this temperature that do not follow the trend, that could be due to measurement errors. Considering this, linear equations were proposed from the obtained parameters at 450°C and 475°C, as a function of air temperature. The parameters at 425°C were found using this linear expressions. The equations are shown in Table 3.

Fig. 4. Effect of air temperature and time on 5-CQA content, and fit to the kinetic model proposed  $dC/dt = -Ae^{B/T_p(t,T_a)}C^n$ .

The fit of the kinetic model using those parameters was acceptable ( $R^2$  of 0.978 and a  $\text{RMSECV}$  of 7.6%). The linear model approach is justified since the range of temperatures in the study is narrow, and also because the interest of this work was to have a generalized model for all the temperature range, and not to only have punctual parameters for the three essayed temperatures. The final fits are illustrated in Fig. 4. It can be appreciated that the kinetic model developed in the present work describes properly the degradation kinetics of chlorogenic acid for the three air temperatures, even though it is more precise at higher temperatures. This graphic evinces the relevance of the time-temperature profiles, and also shows that for a given roasting time, the 5-CQA content decreases as the thermal process intensity increases, as previously reported (Baggenstoss *et al.*, 2008; Moon & Shibamoto, 2009; Schenker, 2000). Also, Fig. 5 proves that there is a good correlation between the experimental and predicted 5-CQA concentrations.

Finally the same optimization algorithm was used to find the parameters and evaluate the goodness of fit of the model of Eq. (4), which considers a constant temperature (air temperature).

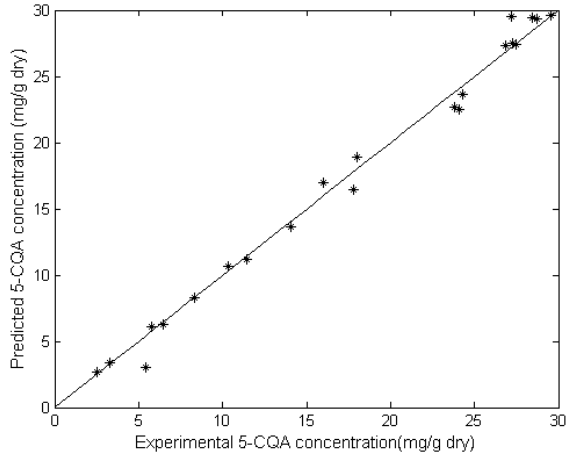


Fig. 5. Comparison between experimental 5-CQA content values and the predicted values by the model.

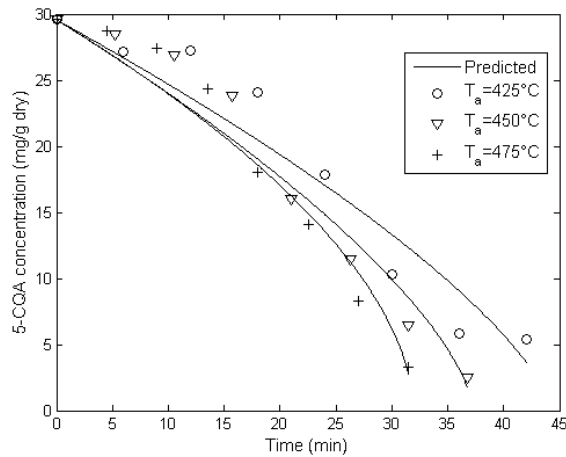


Fig. 6. Fit of an isothermal model dependent on air temperature to the 5-CQA content  $dC/dt = -Ae^{B/T_a}C^n$ .

The bad fit of the model to the experimental values is reflected in the  $R^2$  (between 0.930 and 0.966) and RMSEVC values (between 8.9% and 13.5%). The behavior of the model is exhibited in Fig. 6, where it is clear that the model does not follow the trend of the experimental data; this supports the significance of considering the temperature of the kinetic model as the particle temperature (as function of time), and not the constant air temperature, as previous work had suggested (Perrone *et al.*, 2010). It is clear that the heat transfer resistance between air and beans prevents the bean temperature from being at equilibrium with air temperature since the beginning of the process.

## Conclusions

The kinetic model developed in this work describes properly, with more than a 95% accuracy, the degradation of 5-CQA during coffee roasting in an innovative spouted bed system under the studied conditions. The relevance of considering the process as non-isothermal was proved, given the dependence of 5-CQA content on particle temperature, which changes with time and that is not the same as the air temperature. Future work should be directed towards the development of a semi-empirical model that incorporates phenomenological models to compute bean temperature.

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## Nomenclature

$T_p$	particle temperature, °C
$T_a$	air temperature, °C
$t$	roasting time, min
$A$	parameter of the kinetic model, $\text{min}^{-1}$
$B$	parameter of the kinetic model, °C
$n$	parameter of the kinetic model, (-)
%H	moisture content (g water/g wet coffee)
$C$	chlorogenic acid concentration (mg 5-CQA/g dry coffee)
$p_0$	parameter of the particle temperature model (-)
$p_1$	parameter of the particle temperature model (-)
$p_2$	parameter of the particle temperature model (-)
$q$	parameter of the particle temperature model ( $\text{min}^{-1}$ )
$s$	parameter of the particle temperature model ( $\text{min}^{-1}$ )

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