



Original research

## Prediction of the physicochemical properties of quince puree during thermal treatment using M5 decision tree

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### ABSTRACT

Thermal pasteurization is known as the most common method in food processing. In this study, the effectiveness of come up time on inactivation of heat resistance isoform of polyphenol oxidase (PPO), as a pasteurization index, was investigated during heating of the quince puree in a water bath at 60 to 90°C. M5 decision tree, a novel statistical method, was applied to understand the simple relationship between the treatment conditions (time and temperature) and changes in physicochemical properties of the puree. Browning index and the total color difference increased as a result of PPO inactivation and ascorbic acid degradation. Based on the results of the M5 decision tree models and sensitivity analysis it showed temperature was a more leading factor in the changes of the puree quality.

Keywords: Quince puree, Thermal treatment, Physicochemical properties, M5 decision tree, Sensitivity analysis

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## 1. Introduction

Quince (*Cydonia oblonga mill*) is a golden yellow color, juicy and sweet-sour taste seasonal fruit (Sharma et al., 2011). Because of its strong acidity, astringency and tough texture, this fruit is usually consumed as cooked puree, marmalade and jelly. Quality of the final product is influenced by softening of texture and changes in color during thermal treatment of quince puree (Akbari & Ebrahimpour, 2014).

Ascorbic acid (AA) is known as an indicator of changes in food nutritional value because of its sensitivity to processing conditions such as time and temperature (Lee & Kader 2000). Non-enzymatic browning, as the major factor affecting the color of the quince puree, occurs via the thermal degradation of this vitamin (Burdurlu et al., 2006). Several researchers have studied the effect of different thermal treatment conditions on the alteration of the color in various food products. In thermal treatment methods (IR and conventional), it was shown that the higher temperature and longer process time induce more variation in color of the citrus juice (Aghajanzadeh et al., 2016a; Vikram et al., 2005).

Polyphenol oxidase (PPO, EC 1. 14.18.1), which naturally found in quince, produces browning pigments by oxidizing phenolic compounds (Dalmadi et al., 2006). Hence, PPO inactivation using thermal treatment prevents nutritional loss and

undesirable enzymatic browning. Due to its higher thermal resistant than spoilage microorganisms, it is also known as an indicator during the blanching process of high acid food products (pH < 4.6) (Chen et al., 2004; Vamos-Vigyazo & Haard, 1981; Weng et al., 1991). PPO inactivation followed the first order kinetic model during the microwave processing of green coconut water (Matsui et al., 2008). It was reported that the thermal inactivation of this enzyme in Fuji apple followed zero order kinetic model (Bai et al., 2013). Researchers also studied the effect of temperature on PPO inactivation during the thermal treatment of pineapple puree using water bath (Chutintrasri & Noomhorm, 2006).

Therefore, the combination of time and temperature should be accordingly considered to decrease AA loss and control the undesirable color changes besides PPO inactivation. Since inactivation of enzymes and microorganisms not only occur during holding time but also in come-up time (CUT); effectiveness of CUT should be consequently considered to reduce the needed heating intensity in PPO inactivation. According to Ball (1923), 42% of CUT has the inactivation effect on enzymes and microorganisms. But, some researchers calculated the effectiveness of this stage on enzyme inactivation using time-temperature profile and different equations (Aghajanzadeh et al., 2016b; Tajchakavit & Ramaswamy, 1997).

Statistical decision tree (DT) model is used in the fast exploration of the most simple patterns by summarizing, classifying

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and estimating the data, even in different measurement scales (Saito et al., 2009). In this model, the data with any frequency distributions are represented as a tree structure and the relationships between the independent (inputs) and dependent variables (responses) are briefly extracted (Saito et al., 2009). This model is rarely used in food science but it can be quickly trained and performed unlike neural networks (Pal & Mather, 2003). The main advantages of DT models are related to providing simpler categorized models (linear models). In this model, a “data set” is classified into smaller subdivisions in a tree structure including root (test on an attribute), branches (the outcome of the test), leaves (class label or taken a decision after computing all attributes) and classification rules are shown as paths from the root to leaves (Friedl & Brodley, 1997). Each node makes a binary decision and separates one or more classes from the remaining ones. To increase computational efficiency, features with the maximum information representation are chosen for classification and the remaining features are rejected, thereby increasing computational efficiency (Xu et al., 2005).

The main objectives of this study were to (1) estimate the effectiveness of CUT based on PPO inactivation during thermal treatment of quince puree, (2) calculate the exact required time for thermal treatment of quince puree based on the estimated CUT effectiveness, (3) study the kinetic of PPO inactivation and changes in AA, browning index (BI) and total color difference (TCD), (4) understand the relationship between the thermal treatment conditions (time and temperature) and physicochemical properties of the puree using DT technique and (5) examine the effectiveness of the heating process factors using sensitivity analysis.

## 2. Material and Methods

### 2.1. Preparation of quince puree

Quince fruit (*Cydonia oblonga mill*) was obtained from a local market and was kept in a refrigerator at 4°C until the experiments. The fruit was washed, hand peeled and crushed. The seed and the larger pulps were separated from the crushed quince using a sieve with mesh size 200. A test tube (15 mm outer diameter, 160 mm length and 1 mm thickness) was filled with 15 mL of the sample (11° Brix). The quince puree was immediately heated at 60, 70, 80 and 90°C in a water bath (WNB-22, Memmert, Germany). During heating, the time-temperature data was recorded using a data logger (TC-08, Pichotechnology Co, UK) and a 1 mm diameter copper-constantan thermocouple (T-type) inserted in the sample. The samples were then removed from the water bath and cooled down to 25°C immediately in ice-water.

### 2.2. Analyses of quince puree properties

#### 2.2.1. Chemical properties

pH, total acidity, total soluble solids, moisture content and total ash (dry basis) of fresh quince puree were determined (AOAC, 2012). pH was measured using pH-meter (W3B, BEL, Italy) at 25°C. Total acidity (as %malic acid) was determined using the NaOH 0.1 N solution (titrant) and phenolphthalein (indicator). Total soluble solids (°Brix) were determined by a refractometer (UV/VIS80 +T, PG Instrument, US) at 25°C. Moisture content was measured by drying the sample up to a constant weight at 105 ± 1°C in a hot-air oven (FD53, Binder, Germany). The ash content

was measured by burning the puree at 525°C up to a constant weight.

#### 2.2.2. Measuring the PPO activity

In order to measure the PPO activity, 10 g of puree was mixed with 10 mL of citric-phosphate buffer (pH = 6.5) at 3000 rpm for 1 min (Palou et al., 1999). The homogenized sample was then centrifuged (7000 rpm, 30 min, 4°C) and the supernatant was filtered using Whatman paper (no 1). 1 mL of catechol solution (0.175 mol.L<sup>-1</sup>) and 2 mL of citric-phosphate buffer (pH = 6.5) were added to the filtrate (0.5 mL). The optical density of the solution was measured at 420 nm (T-80, UV/VIS Double Beam Spectrophotometer) every 10 s up to 1 and 2 min in the fresh and treated purees, respectively (Pizzocaro et al., 1993). The obtained data were plotted against time. The PPO activity was calculated from the slope of the initial linear part of the curve and defined as 0.001 ΔA<sub>420</sub> min<sup>-1</sup> (mL of extract)<sup>-1</sup>.

#### 2.2.3. Ascorbic acid content measurement

Based on the iodine titration method, 20 ml of the puree was diluted in 150 ml of distilled water and titrated with iodine solution in presence of 1% starch indicator (Kashyap & Gautam, 2012). The iodine solution was prepared by dissolving 5 g potassium iodide and 0.268 g potassium iodate in 200 ml of distilled water. 30 mL of 3 M sulfuric acid was then added and diluted with distilled water until 500 mL. The final point of the titration was determined by observing a fixed dark-blue color. AA content was estimated using Eq. 1 as 0.88 mg AA equivalent to 1 mL of iodine solution consumption.

$$\frac{\text{mg ascorbic acid}}{100 \text{ mg of the sample}} = 0.88 \times \text{Iodine solution consumption (mL)} \quad (1)$$

#### 2.2.4. Color properties evaluation

In order to measure the BI, the absorbance of the puree was recorded at 420 nm (Ibarz et al., 1999). To analyze the color changes of the puree during heating, 15 mL of sample was filled in a plate (with 1 cm height and 6 cm diameter) and its picture was taken by a scanner (Scanjet G2710, HP, USA) and was saved as JPEG format and 600 dpi resolution (RGB color). To prevent environmental light, the scanner was completely shielded by a black cover. According to image processing method, the taken pictures were analyzed using ImageJ software (version 1.42e, Wayne Rasband, National Institutes of Health, USA) to convert the RGB color space to CIE L\*, a\* and b\* coordinates. These parameters were used to calculate TCD according to Eq. 2 (Ibarz et al., 1999):

$$\text{TCD} = \sqrt{(\Delta L^*)^2 + (\Delta a^*)^2 + (\Delta b^*)^2} \quad (2)$$

where, the ΔL\*, Δa\* and Δb\* refers to the difference between the color parameters of the fresh puree and the treated one.

### 2.3. Modeling

#### 2.3.1. Kinetics modeling

Zero and first-order kinetics model were usually used to describe the thermal inactivation of PPO, AA, BI and TCD (Eq. 3 and 4):

$$A = A_0 - kt \quad (3)$$

$$\ln\left(\frac{A}{A_0}\right) = -kt \quad (4)$$

where A and A<sub>0</sub> are residual and initial values of the defined properties of the quince puree. k shows the constant rate (min<sup>-1</sup>) of inactivation or changes and t represents the process time (min). The calculated constant rates were used to calculate D-value (min) relating to the required time to obtain 90% changes in the physicochemical properties of quince puree (Eq. 5):

$$D = \frac{2.303}{k} \quad (5)$$

The needed temperature to reach 10 folds reduction in D-value is represented by Z-value that is calculated based on the negative slope of D-value vs. temperature (Eq. 6):

$$Z = \frac{T_2 - T_1}{\ln D_1 - \ln D_2} \quad (6)$$

where T<sub>2</sub> and T<sub>1</sub> represent the temperatures corresponding to D<sub>2</sub> and D<sub>1</sub>, respectively. D and Z values were computed from the uncorrected heating times based on the time-temperature profile during CUT. The effectiveness of heating time (t<sub>e</sub>) was calculated using Eq. 7 in which the lethality (L) were computed using the uncorrected Z-value.

$$t_e = \int_0^t L dt = \int_0^t 10^{\frac{T-T_{ref}}{Z}} dt \quad (7)$$

where T<sub>ref</sub> is the reference temperature according to the water bath temperature in each heat treatment. D and Z values were recalculated using the corrected thermal times. The more accurate thermal times were recalculated using the Eq. 7 with the new Z-value. This procedure was repeated until the difference between two sequential Z-values were within 5%. As a final point, the effectiveness of CUT was estimated at each heat treatment temperature by the calculated lethality or thermal time divided by the CUT (Tajchakavit & Ramaswamy, 1997).

### 2.3.2. Decision tree classifiers

In this study, the M5 algorithm was used to combine the features of classification and regression as it is a comprehensive, reproducible and comprehensible method in practical experiments using “Rapid Miner 5” software (version 3). In this method, a conventional DT combines with the linear regression functions at the leaves (Solomatine & Xue, 2004). The M5 tree categorizes between the linear and nonlinear models. A multi-stage or sequential approach is used in DT in classifying the labels.

### 2.3.3. Building model tree

For building the model tree, an attribute (time or temperature) is chosen as the root node; the first branch is then made for each

value. The process is recursively repeated for each branch until all data categorized in the appropriate leaves (Mehta et al., 1996). In DT, the splitting procedure is done according to filtering and categorizing many samples from the same class into one subset (Solomatine & Xue, 2004). Splitting criterion is used for the selection of the attribute in a split for a given set. This statistical property is based on the standard deviation of the values in the subset of the training data which reaches to a specific node. An appropriate attribute, which maximizes the expected error reduction, is selected for splitting at the node. The splitting process continues until a few experimental data remain in a subset and the standard deviation of the output data becomes less than 5% of the standard deviation of the original data (Solomatine & Xue, 2004). The linear regression models are built for each subset associated with the leaves. In this study, the numeric attributes were used in the form of A ≤ v. Where, A and v represent the numeric attribute and real value, respectively.

### 2.3.4. Sensitivity analysis

Sensitivity analysis (SA) examines the uncertain impact of the input factors variation on the output of a numeric model (Eslamian et al., 2011; Pianosi et al., 2016). In this study, the one (factor) at a time (OAT) method was used to study SA. The output variation changes as the input factors alter. In order to examine the SA of the M5 model, one factor was altered by considering the other one constant as following Eq. (8).

$$y = f(x_1, [x_2 + (x_2 \times p)]) \quad (8)$$

where y is the output property, x refers to the inputs variables (time and temperature) and p is the percentage of the alteration in one factor (0 to 50%). The Eq (9) was finally used to evaluate the SA of the M5 model:

$$\text{Sensitivity of the M5 model} = \left| \frac{\text{Experimental value} - \text{Predicted value}}{\text{Experimental value}} \right| \quad (9)$$

### 2.4. Statistical analysis

In this study, completely randomized design was used to investigate the effect of temperature and time of heating treatment on PPO activity, AA content and variation of BI and TCD, using SAS software (version 9.1). All experiments were performed twice and the presented results are the mean of the obtained value ± standard deviation. Results were submitted to analysis of variance (ANOVA) with a significance level of p < 0.05. Microsoft Excel 2010 was also used to create the charts and represent the results.

Minitab software (version 17) was also used to describe the polynomial relationship between the thermal treatment conditions and the physicochemical properties of the puree. The accuracy of the predicted models was investigated based on the correlation coefficient (R<sup>2</sup>) and Root Mean Square Error (RMSE) using Eqs. 10 to 11:

$$R^2 = 1 - \frac{\sum_{i=1}^n (x_{pi} - x_{ei})^2}{\sum_{i=1}^n (x_{pi} - \bar{x})^2} \quad (10)$$

$$RMSE = \sqrt{\frac{1}{n} \sum_{i=1}^n (x_{pi} - x_{ei})^2} \quad (11)$$

where,  $x_{pi}$  and  $x_{ei}$  are the predicted and experimental value of the physicochemical properties of quince puree (PPO activity, AA content, BI and TCD), respectively.  $\bar{x}$  indicates the average of the experimental value and  $n$  indicates the total number of all observations. In addition, student's t-test was also performed between the experimental and predicted values to evaluate the predicted polynomial regression and M5 models with a significance level of  $p < 0.05$  (Eq. 12).

$$t = \frac{|\bar{x}_e - \bar{x}_p|}{\sqrt{\frac{S_e^2}{n_e} + \frac{S_p^2}{n_p}}} \quad (12)$$

Subscripts of e and p indicate the experimental and predicted values, respectively.  $\bar{x}$ ,  $s^2$  and  $n$  are mean, variance and number of data, respectively.

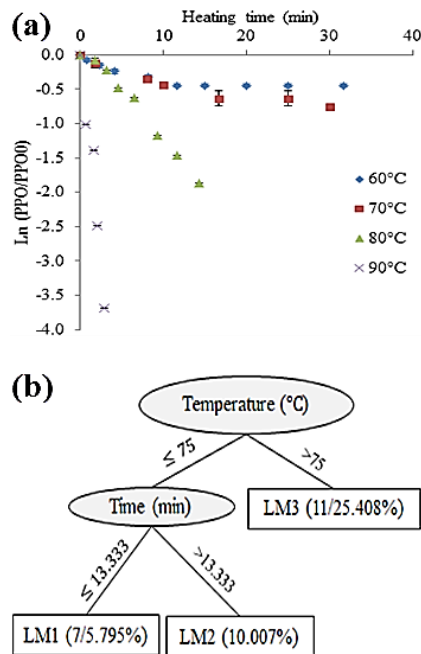


Fig. 1. (a) Thermal kinetics and (b) decision tree for classifying of PPO inactivation during heating treatment of quince puree at different temperatures.

Table 1. Constant rate and D-values of inactivation of PPO heat resistance isoform during thermal processing.

Temperature (°C)	Constant rate (min <sup>-1</sup> )	R <sup>2</sup>	D-value (min)
60	0.004	0.98	523.41
70	0.006	0.90	390.34
80	0.059	0.98	38.84
90	0.485	0.91	4.75

### 3. Results and Discussion

#### 3.1. Polyphenol oxidase thermal inactivation

The pH, acidity (malic acid), total soluble solids, moisture content and ash (dry basis) of the fresh puree were  $3.92 \pm 0.04$ ,  $0.8 \pm 0.2\%$ ,  $13.2 \pm 0.2$  °Brix,  $86.46 \pm 0.06\%$  and  $0.34 \pm 0.02\%$ , respectively. Considering the pH of this high acid puree, heat treatment below 100°C can be used in order to guarantee its safety.

Fig. 1a shows the thermal inactivation of PPO during the heating of the quince puree at different temperatures. PPO inactivation increased significantly at a higher temperature and longer process time ( $p < 0.05$ ). In the samples treated at 60 and 70°C, the enzyme inactivation curve was nonlinear, showing the presence of various PPO isoforms with different thermal resistances (Yemenicioglu et al., 1999). Heat sensitive and heat liable isoforms could be recognized by separating these curves into two first-order rates (linear) curves. Therefore, the heat-sensitive isoform showed rapid inactivation even at these temperatures. At higher temperatures (80 and 90°C), the heat-sensitive isoform was already inactivated during CUT; hence, only the inactivation of heat resistance isoform is observed during the holding time. These results are in agreement with other researchers reported that the heating conditions and type of fruits or vegetables influence on a variety of PPO isoforms (Bai et al., 2013; Yemenicioglu et al., 1999).

In this study, only the thermal inactivation of the heat resistant fraction of PPO could be studied during holding time. As represented in Table 1, the D-value of heat resistance isoform decreased at higher temperatures. The calculated Z-value of this isoform was 14.26°C ( $R^2 > 0.92$ ), revealing its high thermal resistance. Studies showed that the heat-stable isoform of PPO in Taro was equal to 25.5°C during heating treatment between 60 to 80 °C (Yemenicioglu et al., 1999). Mutsui et al. (2008) calculated the Z-value of PPO in green coconut water equal to 17.6°C during microwave thermal treatment. This value was calculated 23.7 and 82.8°C during thermal processing of pineapple puree at a temperature range of 40 to 70°C and 70 to 90°C, respectively (Chutintrasri & Noomhorm, 2006).

Based on the temperature changes of the puree and using Eq. 7, the effectiveness of CUT on inactivation of heat resistance isoform of this enzyme were calculated as 44.44%, 64.91%, 69.74% and 76.28% respectively at 60, 70, 80 and 90°C, by considering the reference temperature equal 80°C. In this study, 1D reduction in PPO activity was used for the optimization and calculation of the adequate heating time at different temperatures; since its activity is introduced as pasteurization index (Chen et al., 2004). Using Eq. 7, the needed times for thermal treatment of quince puree were estimated 77.93, 33.48, 16.1 and 7.16 min respectively at 75, 80, 85 and 90°C. This range of temperature was selected as too long processing time would be needed based on the calculated D-values at lower temperatures (60 and 70°C).

The relationship between the thermal treatment conditions (time and temperature) and PPO inactivation (ratio of PPO activity in treated puree to the fresh one) was determined by a polynomial regression model (Eq. 13). According to the estimated statistical parameters, the regression coefficient and RMSE of this model were 0.65 and 0.18, respectively. In this Equation, the inverse relationship between the PPO activity, time and temperature were represented by negative coefficients. Based on t-test, there was no significant difference between the experimental percentages of the PPO activity and the predicted ones using Eq. 13 ( $p > 0.05$ ).

$$\begin{aligned} \text{Ratio of PPO activity (\%)} &= (-2.216 \times \text{Temperature}) \\ &\quad - (1.295 \times \text{Time}) + 231 \end{aligned} \quad (13)$$

Based on the M5 model tree, three leaf nodes were generated, each one representing the linear model to predict the PPO inactivation (Fig. 1b). LM1 and LM2 respectively represented the models for heating at lower than 75°C for equal or less than 13.33 min and more than 13.33 min. The predicted linear models are presented with a high correlation coefficient ( $R^2=0.86$  and  $RMSE = 0.10$ ) as LM1 to LM3 (Eqs. 14 to 16). Based on the coefficients of the models, it could be concluded that at the temperature higher than 75°C (LM 3), the effect of temperature was about 3.12 times greater than heating at a lower temperature ( $\leq 75^\circ\text{C}$ ). In addition, it can be concluded that processing time had a more intensive effect on the inactivation of the PPO when the puree was treated at a higher temperature. Statistical analysis revealed that there is no significant difference between the experimental data and predicted ones using M5 tree models ( $p > 0.05$ ).

$$\begin{aligned} \text{LM1: Ratio of PPO activity (\%)} \\ &= (-1.3298 \times \text{Temperature}) \\ &\quad - (1.5396 \times \text{Time}) + 174.1038 \end{aligned} \quad (14)$$

$$\begin{aligned} \text{LM2: Ratio of PPO activity (\%)} \\ &= (-1.3298 \times \text{Temperature}) \\ &\quad - (1.2753 \times \text{Time}) + 1708979 \end{aligned} \quad (15)$$

$$\begin{aligned} \text{LM3: Ratio of PPO activity (\%)} \\ &= (-4.1536 \times \text{Temperature}) \\ &\quad - (3.432 \times \text{Time}) + 404.5349 \end{aligned} \quad (16)$$

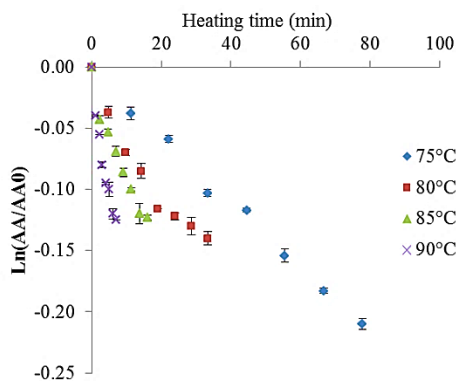


Fig. 2. Inactivation kinetic of Ascorbic acid during thermal processing of quince puree at 75 to 90°C.

Table 2. Constant rate and D-value of ascorbic acid degradation during quince puree thermal treatment

Temperature (°C)	Constant rate ( $\text{min}^{-1}$ )	$R^2$	D-value (min)
75	0.003	0.99	852.96
80	0.004	0.93	548.33
85	0.007	0.96	324.37
90	0.017	0.94	139.58

### 3.2. Kinetic of ascorbic acid degradation

Fig. 2 shows that AA content was significantly reduced as the time and temperature increased ( $p < 0.05$ ) during the quince puree thermal treatment. The AA degradation followed the first order

kinetic model with a high correlation coefficient ( $R^2 > 0.95$ ) (Aghajanzadeh et al., 2016; Bai et al., 2013). Based on the obtained slope of each curve in Fig. 2, the constant rates of AA degradation were calculated ( $R^2 > 0.93$ ). The obtained data revealed that these values rise at higher temperatures showing the thermal sensitiveness of this vitamin (Table 2). Vikram et al. (2005) reported that the D-value of AA is reduced as temperature increased during orange juice thermal treatment using different thermal methods including conventional heating in a water bath, ohmic heating, microwave and infrared irradiation. It could be concluded that applying different processing methods (with different CUT and intensities) have dissimilar effects on AA degradation.

Z-value was estimated  $19.34^\circ\text{C}$  by plotting the D-values vs. temperature ( $R^2 > 0.97$ ). Vikram et al. (2005) reported that Z-value of AA was between  $19.23$  and  $26.25^\circ\text{C}$  during thermal treatment of orange juice using electromagnetic and conventional methods. The Z-values of AA degradation in key lime juice treated by conventional and infrared heating were  $24.15$  and  $25.12^\circ\text{C}$ , respectively (Aghajanzadeh et al., 2016).

Eq. 14 represents the obtained polynomial regression model ( $R^2 > 0.81$  and  $RMSE = 0.02$ ) to describe the linear relationship between the thermal treatment conditions and percent of the AA preservation ratio in the heated product in comparison to the fresh puree. Using the DT method, one linear model (exactly like Eq. 17) was generated for prediction the changes of AA content during thermal treatment. This model revealed that the applied temperature had a stronger effect (1.73 times) on AA degradation rather than heating time. There was no significant difference between the experimental AA contents and the predicted ones using this model ( $p > 0.05$ ). Therefore, this model can be effectively used to predict the AA content in quince puree during heating treatment.

$$\begin{aligned} \text{AA preservation ratio (\%)} \\ &= (-0.4195 \times \text{Temperature}) \\ &\quad - (0.2422 \times \text{Time}) + 129.9553 \end{aligned} \quad (17)$$

### 3.3. Color changes

#### 3.3.1. Changes in browning index

As shown in Fig. 3a, BI of the quince puree increased following the first-order kinetic model during heating ( $p < 0.05$ ). Rising in BI can be related to the enzymatic browning (PPO activity) and non-enzymatic browning (AA degradation). At higher temperatures, the changes in BI were lower due to more PPO inactivation and lower AA degradation. During processing the juice with high AA content, the maximum level of non-enzymatic browning was detected when the vitamin was in the minimum level (Roig et al., 1999). Rising in BI results in decreasing in lightness, rising in reddish color tone, deterioration of aroma and flavor and finally have adverse effects on quality and acceptance of the processed food (Aghajanzadeh et al., 2016; Avila & Silva, 1999).

Eq. 18 ( $R^2 > 0.77$  and  $SE = 0.07$ ) was developed in order to predict the relationship between the thermal processing conditions and alteration in BI of the treated vs. the fresh quince puree (percent of BI changes ratio). There was no significant difference between the predicted value using this model and the experimental ones ( $p > 0.05$ ). According to this regression model, the temperature had about 1.17 times the higher effect on BI alteration.

Positive coefficients revealed the increase in BI during thermal treatment at a higher temperature during a longer process time.

$$\begin{aligned} \text{Ratio of BI changes (\%)} &= (0.902 \times \text{Temperature}) \\ &- (0.7678 \times \text{Time}) + 47.3 \end{aligned} \quad (18)$$

Using the DT method, based on the classification of the heating time, the change in BI could be predicted using two suggested M5 tree models (Fig. 3b). Considering the performance of the models ( $R^2 = 0.93$  and  $RMSE = 0.05$ ), it can be concluded that these models are more appropriate in the prediction of the BI alteration during thermal treatment of the quince puree than Eq.15. Considering the coefficients of the linear regressions (Eqs. 19 and 20), the effect of temperature on BI variation was 1.34 times higher when the product heated over 23.05 min (LM2). This fact can be related to the lower PPO inactivation and also higher AA degradation at below 80°C as a result of longer heating time. The result of statistical evaluation revealed that there was no considerable difference between the experimental and predicted values using LM1 and LM2 models ( $p > 0.05$ ).

$$\begin{aligned} \text{LM1: Ratio of BI changes (\%)} &= (1.3093 \times \text{Temperature}) \\ &- (1.2571 \times \text{Time}) + 79.541 \end{aligned} \quad (19)$$

$$\begin{aligned} \text{LM2: Ratio of BI changes (\%)} &= (1.7518 \times \text{Temperature}) \\ &- (0.7097 \times \text{Time}) + 14.4621 \end{aligned} \quad (20)$$

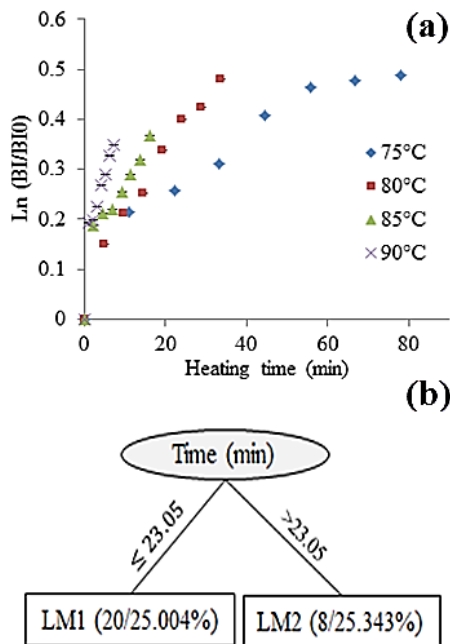


Fig. 3. (a) Thermal kinetics and (b) decision tree for classifying of the alterations in browning index during heating treatment of quince puree at different temperatures.

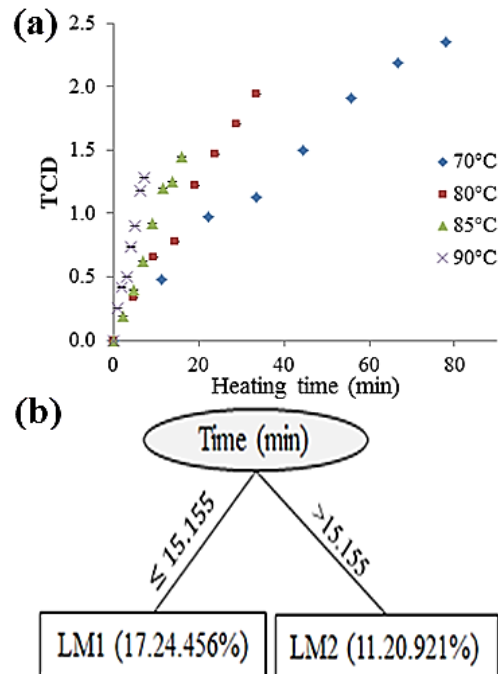


Fig. 4. (a) Thermal kinetics and (b) decision tree for classifying of total color difference (TCD) during heating treatment of quince puree at different temperatures.

### 3.3.2. Total color difference alteration

The total color difference (TCD) is considered as an appropriate index to evaluate the changes in the color of food products (Avila & Silva, 1999). Like BI, the calculated TCD were lower at higher temperatures and also a shorter process (Fig. 4a). The statistical analysis of the obtained results showed that thermal treatment conditions had a significant effect on TCD variation ( $p < 0.05$ ). According to Eq. 21, the temperature had 1.61 times more intensive effect on changes in TCD rising than the time of heating ( $R^2 > 0.78$  and  $SE = 0.29$ ). There was no significant difference between the predicted TCD using this linear model and the experimentally measured values ( $p > 0.05$ ).

$$\text{TCD} = (0.033 \times \text{Temperature}) + (0.0205 \times \text{Time}) - 2.27 \quad (21)$$

As shown in Fig. 4b, the TCD changes were classified into two categories based on the time of heating. The suggested M5 models (Eqs. 22 and 23), having the correlation coefficient and RMSE 0.90 and 0.18, respectively. In the LM1 model, the temperature coefficient was the same as its coefficient for the processed puree for longer than 15.155 min. These models are useful in TCD prediction since there was no significant difference between the experimental and predicted TCD ( $p > 0.05$ ).

$$\begin{aligned} \text{LM1: TCD} &= (0.0516 \times \text{Temperature}) + (0.0673 \times \text{Time}) \\ &- 4.1377 \end{aligned} \quad (22)$$

$$\begin{aligned} \text{LM2: TCD} &= (0.0551 \times \text{Temperature}) + (0.0299 \times \text{Time}) \\ &- 3.8611 \end{aligned} \quad (23)$$

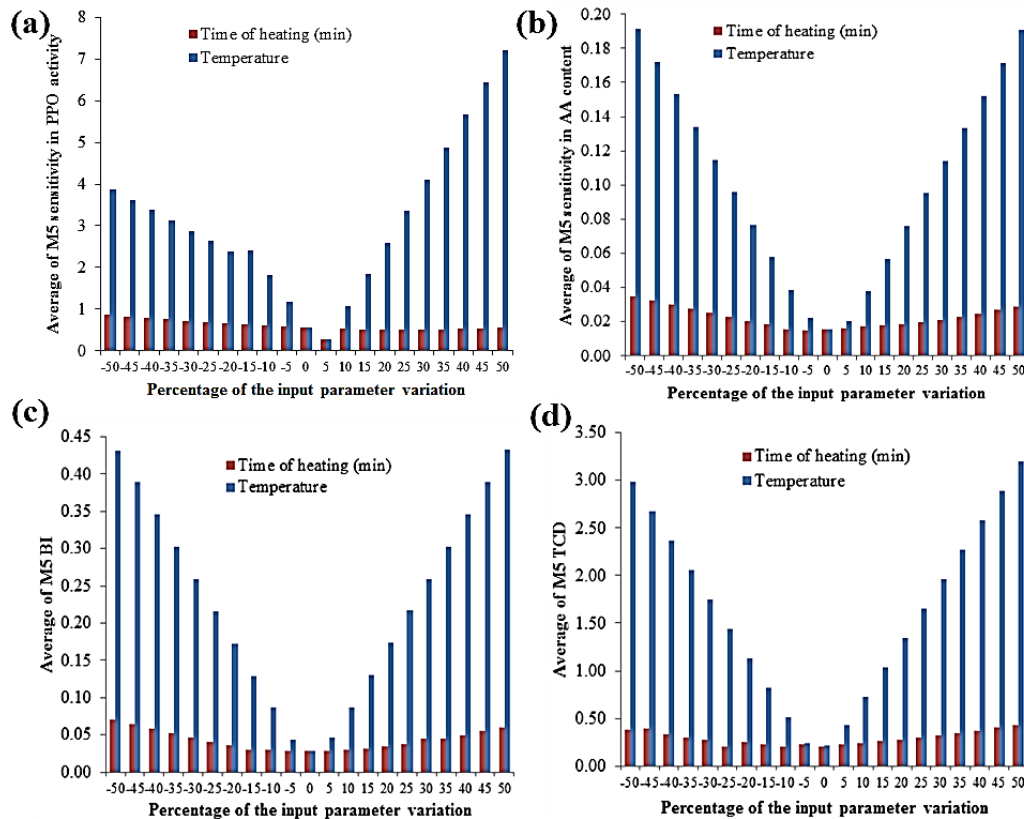


Fig. 5. Sensitivity analysis of (a) PPO activity, (b) AA retention, (c) BI alteration and (d) TCD changes during the quince puree processing based on the M5 model.

### 3.4. Sensitivity analysis

As shown in Fig. 5a, the ratio of the PPO activity changed considerably at different temperatures. Variation in the temperature during the heating process of the quince puree is therefore efficient in controlling of the PPO inactivation up to the desired value. It was also revealed that AA degradation had a lower sensitivity to the temperature rather than the time of heating (Fig. 5b). Hence, controlling the temperature during thermal treatment is more essential than adjusting the process time in order to prevent the high loss of this vitamin. It was also observed that temperature had the higher effect on the BI and TCD changes in comparison to the time of heating (Fig. 5c and d), which are directly related to the intensive influence of the applied temperature on PPO activity and AA content. By this way, prevention from increasing of the BI and TCD changes during heating of the quince puree could be achieved more easily by controlling the applied temperature.

## 4. Conclusion

The effect of thermal treatment on the PPO activity of quince puree was studied during conventional treatment using a water bath. As the heat-sensitive isoform inactivated completely at higher temperatures than 80°C, thermal inactivation of the heat resistant fraction of PPO was investigated during the holding time. Based on the calculated Z-value of heat resistance isoform, the effectiveness of CUT on inactivation of heat resistance isoform of PPO was estimated for the optimization and calculation of the adequate pasteurization time at 75 to 90°C. The degradation of AA was

studied in these predicted conditions and the obtained results showed that the AA content decreased during thermal processing following the first order kinetics model. During thermal treatment, the BI and TCD increased as a result of occurring enzymatic and non-enzymatic browning reactions. DT method was successfully used as a helpful and novel method in the classification of the studied physicochemical properties of the quince puree. The DT structures revealed a clear description of the relationship between inputs parameters (temperature and time) and the physicochemical properties of the puree. The higher performance of M5 models than the polynomial regression model was confirmed using statistical analysis. Based on the results of the sensitivity analysis, the temperature was the dominant factor in the PPO inactivation, AA degradation, BI alteration and rising in TCD as compared to the heating time. Considering the simplicity and high accuracy M5 models, further studies should be performed to develop the application of M5 decision tree method in food science.

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