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Modeling respiration and transpiration rate of minimally processed pineapple (*Ananas comosus*) depending on temperature, gas concentrations and geometric configuration

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This study presents a mathematical model to describe respiration (O2 consumption and CO2 production) and transpiration rates of minimally processed pineapple (cut into slices) as a function of temperature, relative humidity (RH) and geometric configuration. To experimentally adjust suitable models for respiration and transpiration, minimally processed pineapple (*Ananas comosus*) was stored in slices of three types of configuration (a complete slice with 1 centimeter of thickness, a complete slice with 2 centimeter of thickness and a half slice with 1 centimeter of thickness) at different temperature and RH. To estimate respiration rates, two possible models were compared and the most suitable one was chosen: the O2 consumption and CO2 production were modeled by using a Michaelis-Menten enzyme kinetics and by using a first-order kinetics choosing the former. Throughout the different experiments, the respiration rates were higher by increasing the storage temperature. The transpiration data shows the weight loss is linear for all the samples during the entire storage time. Transpiration was represented by considering the mass transfer (of moisture) due the water activity gradient between the produce and the atmosphere surrounding it, and the water evaporated as a consequence of absorbing the respiratory heat generated in the cut fruits. Results shows a high goodness of fit between experimental data and estimated values with the respiration-transpiration models (R2adj > 0.88).

* 1. Introduction

Minimally processed products represent an important challenge to the postharvest sector because of the difficulty to preserve their nutritional and sensory quality during the commercialization. It is important to know the respiration and transpiration rates to determine the favorable gas (O2 and CO2) levels and relative humidity for a suitable modified atmosphere packaging (MAP). The above considering that inappropriate control of the packaging conditions may lead to undesirable results such as microbial growth, moisture condensation, accelerated physiological decay and shortened shelf life (Song et al., 2002; Sortino et al., 2017). Respecting high perishable produce such as pineapple (moreover minimally processed), it is very desirable to establish constant and acceptable gas-temperature conditions to preserve its own nutritional and sensory qualities and to avoid rapid decay and deterioration. A number of mathematical models have been proposed to describe a MAP system and to establish favorable gas levels (Benítez et al., 2012; Finnegan et al., 2013). However, as far as it is known, scarce information is available to describe MAP (and specifically respiration-transpiration rates) for minimally processed fruits and for pineapple particularly. By knowing the respiration and transpiration rates depending on storage and packaging conditions, it could be possible to improve the postharvest handling and reduce losses for this fruit that has been one of the most consumed tropical fruits in the world.

Therefore, the aim of this study was to propose mathematical models to represent O2 consumption, CO2 production and transpiration (water vapor generation) rates of sliced pineapple depending on temperature, gas concentration and cutting configuration.

* 1. Materials and methods

Fruits

Pineapples (*Ananas comosus*) MD2 were provided by a local fruit store in Bogotá, Colombia the evening before each trial and stored at 12 °C up to 16 hours until minimal processing. Samples without evidence of damage were selected, cleaned with potable water and left to dry (surface water) at room temperature before the processing stage.

Fruit processing

The pineapple crown and peels were removed manually by using a clean stainless-steel knife. Three types of configuration were cut: a complete slice of one-centimeter thickness and 10-centimeter diameter approximately, a complete slice of two-centimeter thickness and a half of a slice of one-centimeter thickness.

Determination of the respiration rates

The respiration rates (O2 consumption and CO2 generation) of the minimally processed pineapple were determined by using a closed system method (Castellanos et al., 2016a). Two samples of each pineapple slices configurations, previously described, were placed in a hermetic container of 2176 cm3 separated by a grid of 5- centimeter height. The O2 and CO2 concentrations were determined with an electronic analyzer Oxybaby® 6i (WITT-Gasetechnik GmbH & Co KG, D-58454 Witten, Germany). The tests were performed in cabinets with controlled temperature at 8, 12.5, 17 and 21 ± 0.5°C and taking measurements every 2.5 hours until reaching an O2 concentration of 5%. All the measurements for each configuration were performed in triplicate and reporting the average value of each measurement.

The respiration rates were calculated at each temperature by using the following equations:

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| $$r\_{O\_{2}}\left(t\right)=\left(\frac{V}{W}\right)\left(\frac{y\_{O\_{2}t-1}-y\_{O\_{2}t+1}}{∆t}\right)$$ | (1) |
| $$r\_{CO\_{2}}\left(t\right)=\left(\frac{V}{W}\right)\left(\frac{y\_{CO\_{2}t+1}-y\_{CO\_{2}t-1}}{∆t}\right)$$ | (2) |

Where $r\_{O\_{2}}\left(t\right)$ and $r\_{CO\_{2}}\left(t\right)$ are the respirations rates at time $t$ (cm3 kg-1 h-1), $V$ is the free package volume (cm3), $W$ is the slice weight (kg) and $∆$t is the time pass between two consecutive measurements (h). $y\_{O\_{2}t-1}$, $y\_{CO\_{2}t-1}$are the O2 and CO2 mole fractions in the preceding measurement than the time $t$ and $y\_{O\_{2}t+1}$, $y\_{CO\_{2}t+1}$are the following measurement than the time $t$.

Determination of the transpiration rates

The transpiration rates were estimated measuring the experimental weight loss of the minimally processed pineapple configuration slices, described above, using open trays. The change in the sample weight was measured using an Ohaus analytical balance PA-3102 (OHAUS Corp. Pine Brook, NJ, USA). The samples were stored in a Sanyo-Panasonic MLR-352H-PE cabinet (SANYO Electric Co., Osaka, Japan) with controlled temperature and relative humidity, at 8, 12.5 and 17 ± 0.3°C, and at 60, 70, 80 and 90 ± 0.1% RH. The weight measurement was performed every 3 hours for 36 hours. All the samples configurations were performed in triplicate and presenting the average of each measurement.

Transpiration rate was calculated at each temperature using the following equations:

|  |  |
| --- | --- |
| $$r\_{H\_{2}O}\left(t\right)=\frac{W\_{t-1}-W\_{t+1}}{W\_{t}∆t}$$ | (3) |

Where $r\_{H\_{2}O}\left(t\right)$ is the transpiration rate at time t (kg kg-1 h-1), $∆$t is the time pass between two consecutive measurements (h) and $W\_{t}$ is the slice weight (kg). $W\_{t-1}$ the weight in the preceding measurement than the time t and $W\_{t+1}$ is the following measurement (kg) than the time t.

Modeling the respiration rates

Fruit respiration has been described by using mathematical equations to model biochemical systems because of their appropriate representation of the nature of the process and good fit of experimental data (Castellanos et al., 2016a). Between these equations are relevant the Michaelis-Menten equations based on the enzyme kinetics principle and the Chemical Kinetics equations based on the apparent reaction order.

The Michaelis-Menten Kinetics (MM) equation is based on one limiting enzymatic reaction in which the substrate is O2. The respiration rate, $r\_{O\_{2}}$, is (Fonseca et al., 2002; Heydari et al., 2010):

|  |  |
| --- | --- |
| $$r\_{O\_{2}}= \frac{r\_{O\_{2}}^{max}y\_{O\_{2}}}{K\_{m}+y\_{O\_{2}}}$$ | (4) |

Likewise, the Chemical Kinetics (CK) equation is considered to explain the effect of O2 and CO2 concentrations on the respiration rates (Wang et al., 2009):

|  |  |
| --- | --- |
| $$r\_{O\_{2}}=k\_{O\_{2}}y\_{O\_{2}}^{a\_{O2}}$$ | (5) |

Similar equations for MM and CK could be described for the CO2 production rate, also as a function of $y\_{O\_{2}}$.

To determine the respiration rate models (O2 consumption and CO2 production) of minimally processed pineapple, the Michaelis-Menten enzyme kinetics (MM) and the chemical kinetics (CK) equations were used. The experimental data of $r\_{O\_{2}}$, $r\_{CO\_{2}}$, $y\_{O\_{2}}$ and $y\_{CO\_{2}}$ at each temperature were replaced in the linearized form of the MM and CK equations to obtain the model parameters by multiple linear regressions. The models regressions were compared by the adjusted coefficient of determination R2adj (Spiess et al., 2010) that allows the comparison between non-linear models.

The temperature-influence was estimated by adjusting the parameters of each equation in the linearized form of the Arrhenius equation obtaining the pre-exponential factors and the activation energies for each parameter (Castellanos et al., 2017).

Modeling the transpiration rates

Considering that the transpiration process could be described as the water loss in the product because of evaporation (heat transfer) and because of the concentration differences between the product and the surrounding atmosphere (mass transfer) (Castellanos et al., 2016b), the following equation can be written:

|  |  |
| --- | --- |
| $$r\_{H\_{2}O}=\frac{q}{λ}+k(a\_{wp}-a\_{wat})$$ | (6) |

Where $r\_{H\_{2}O}$ is the transpiration rate (kgkg-1 h-1), $q$ is the respiratory heat (kJ kg-1 h-1), $λ$ is the latent heat of moisture evaporation (kJ kg-1), $k$ is the total mass transfer coefficient (kgkg-1 h-1), $a\_{wp}$ is the water activity in the product and $a\_{wat}$ is the water activity in the surrounding atmosphere (RH/100).

Model assumptions and numerical solution

For the development and use of the models the next assumptions were made: the product is in thermal equilibrium with the atmosphere surrounding, the temperature dependent processes can be modelled using the Arrhenius’ law, the respiration and transpiration processes of the product are not affected by the ripening, inside the package there is no stratification of the gases, the system pressure corresponded to the atmospheric pressure and the product not regain the water lost.

* 1. Results and discussion

Respiration rates

Figure 1 presents the respiration rate (O2 consumption, $r\_{O\_{2}}$) of the minimally processed samples and for the three types of geometrical configurations, as a function of O2 inside the hermetic containers (values estimated using Eq. (1) and Eq. (2)). As the figure shows, the O2 consumption rate decrease at lower levels of O2 in the container headspace. The respiration rate measured for the one-centimeter half configuration was higher than the other two configurations (1x1 cm and 1x2 cm) at the same temperature. Possibly, the above is due the additional cut made in the pineapple sample that can induce increasing in respiration as a consequence of the additional injury (Artés-Hernández et al., 2007). Additionally, the one-centimeter slice has a higher O2 consumption rate than the two-centimeter slice at the same temperature, in this case due the higher surface area/weight ratio in the former.

Likewise, the respiratory behavior of the minimally processed samples was described by using the MM and CK equations showing the adjusted values for the O2 production and CO2 consumption rates in Figure 1. These values were calculated using the Eq. (4) and Eq. (5).

The temperature-dependence of the MM parameters (rmax and Km) and of the CK parameters (k) was estimated by using the Arrhenius equation. The respective parameters (pre-exponential factors and activation energies) were determined by linear regression and are shown in Table 1. The positive values in the activation energies for all the parameters shows a direct relationship among temperature and respiration rates. The apparent reaction order (*a*) in the CK equation probed to be temperature-independent.



Figure 1: O2 consumption rate of the three slice-configuration (1/2x1 cm, 1x1 cm and 1x2 cm) as a function of O2 concentration at 8 °C, 12.5 °C and 17 °C. Symbols represent experimental data and lines represent the predicted values using the Michaelis-Menten (---) and Chemical Kinectics (- - -) equations.

By comparing the adjusted coefficients of determination R2adj for each of the respiration models it was found that both (MM and CK) adequately represent the respiratory behavior of the minimally processed pineapple for the different evaluated temperatures. Other studies have demonstrated that the respiration of fresh-cut fruits correspond to an enzymatic process (Lee et al., 1996; Peppelenbos et al., 1996), for this reason the Michaelis-Menten enzyme equation is more appropriate to represent this process. This affirmation is confirmed by the work carried out by Benitez et al. (Benítez et al., 2012).

Table 1: Estimated parameters for O2 consumption and CO2 production rates of the one-centimeter slice, two- centimeter slice and one-centimeter half slice for Michaelis-Menten enzyme (MM) and for Chemical Kinetic equations.

|  |  |  |  |
| --- | --- | --- | --- |
| Model | ½ x 1 cm slice | 1 x 1 cm slice | 1 x 2 cm slice |
| O2 | CO2 | O2 | CO2 | O2 | CO2 |
| *Michaelis-Menten Eq.* |  |  |  |  |  |  |
| rmax (cm3 kg-1 h-1) |  |  |  |  |  |  |
| rmax-ref (cm3 kg-1 h-1) | 1.09±0.03x1022 | 1.91±0.10x1023 | 3.27±0.07x1017 | 9.17±0.34x1019 | 1.45±0.02x1017 | 6.12±0.37x1025 |
| Ea (kJ mol-1) | 109.94 ± 2.75 | 119.46 ± 6.33 | 88.67 ± 1.77 | 103.50 ± 3.83 | 86.96 ± 1.48 | 135.39 ± 8.12 |
| Km  |  |  |  |  |  |  |
| Km-ref | 640.80 ± 16.02 | 1.34±0.07x1010 | 33.02 ± 0.66 | 1.76 ± 0.65 | 43.57 ± 0.74 | 7.31±0.44x1010 |
| Ea (kJ mol-1) | 15.33 ± 0.38 | 59.24 ± 3.14 | 13.73 ± 0.27 | 9.07 ± 0.34 | 14.35 ± 0.24 | 65.92 ± 3.95 |
| R2adj | 0.973 | 0.883 | 0.948 | 0.970 | 0.903 | 0.938 |
|  |  |  |  |  |  |  |
| *Chemical Kinetics Eq.* |  |  |  |  |  |  |
| *A* | 0.87 ± 0.02 | 0.57 ± 0.03 | 0.50 ± 0.01 | 0.27 ± 0.01 | 0.54 ± 0.01 | 0.41 ± 0.02 |
| *k (cm3 kg-1 h-1)* |  |  |  |  |  |  |
| kref (cm3 kg-1 h-1) | 9.90±0.25x1020 | 6.10±0.32x1021 | 1.48±0.03x1020 | 8.87±0.33x1021 | 1.72±0.03x1018 | 4.21±0.25x1027 |
| Ea (kJ mol-1) | 104.79 ± 2.62 | 110.35 ± 5.85 | 101.98 ± 2.04 | 113.45 ± 4.20 | 91.58 ± 1.56 | 144.37 ± 8.66 |
| R2adj | 0.965 | 0.996 | 0.947 | 0.998 | 0.932 | 0.921 |

Rmax: maximum respiration rate (O2 consumption or CO2 production); rmax-ref: maximum rate, pre-exponential factor; Km: Michaelis-Menten constant; Km-ref: Michaelis-Menten constant, pre-exponential factor; a: apparent reaction order; k: rate coefficient; kref: rate coefficient, pre-exponential factor; Ea: apparent activation energies; R2adj: adjusted coefficient of determination.

Transpiration rates

The transpiration rates of the minimally processed pineapple for the different configurations were calculated from the cumulative weight loss data (Eq. (3)). As shown in Figure 2, the samples weight loss increases linearly during the storage time. The fruit weight loss was greater by increasing the storage temperature, being the highest at 17 °C. After 30 hours of storage, the weight loss of the samples stored at 17 °C was 2 times higher than that of the product stored at 8 °C at the lowest relative humidity. In addition, the weight loss for the cut fruits was greater as the relative humidity of the atmosphere surrounding the slices was lower. This because a greater difference in water activity between the samples and the atmosphere results in a high driving force for water evaporation (Becker et al., 2001).



Figure 2: Cumulative weight loss for the pineapple slices stored in open trays at 8 °C, 12.5 °C and 17 °C. The symbols represent experimental data and the lines represent weight loss predicted by model.

With the experimental the transpiration rates estimated at every temperature and slice-configuration and by using Eq. (6), it was possible to obtain coefficients of mass transfer (k) and the fraction of respiratory heat absorbed to evaporate water (*α*) in the cut fruits for each combination temperature and slice-configuration. Then, with the mass transfer coefficients calculated at each temperature, the temperature-dependence was determined by using the Arrhenius equation estimating the parameters performing a linear regression for every slice configuration. In addition, the fraction of respiratory heat turned out to be independent of the temperature.

The overall transpiration model has a high goodness of fit respecting the experimental values measured with R2adj higher than 0.95. These data are shown in Table 2.

Table 2: Parameters for the calculation of the transpiration rate based on the respiratory heat and the water activity difference.

|  |  |  |  |
| --- | --- | --- | --- |
| Configuration | ½ x 1 cm slice | 1 x 1 cm slice | 1 x 2 cm slice |
| Respiration heat |  |  |  |
| α | 0.64 ± 0.03 | 0.68 ± 0.03 | 0.58 ± 0.03 |
|  |  |  |  |
| Mass transfer due the water partial pressure difference |
| *k (cm3 kg-1 h-1)* |  |  |  |
| kref (cm3 kg-1 h-1) | 116333.72 ± 4071.68 | 499298.50 ± 14978.96 | 7162.47 ± 250.69 |
| Ea (kJ mol-1) | 38.65 ± 0.96 | 42.51 ± 1.06 | 33.14 ± 0.83 |
| R2adj | 0.996 | 0.954 | 0.950 |

kref: reference mass transfer coefficient, pre-exponential factor; Ea: apparent activation energies.

The mathematical models described in this study to represent the behavior of the respiration and transpiration rates could be very useful to set specific equilibrium concentration of O2 and CO2, and weight loss by properly modifying the configuration package and storage conditions.

* 1. Conclusions

Experimental measurements show that higher area/weight relation, higher temperature and higher O2 concentration leads to greater respiration and transpiration rates in the cut pineapple. In addition, was observed that extra cuts in the pineapple slices accelerated its metabolic processes.

The proposed models were adjusted satisfactorily to the data obtained experimentally and they can be used to predict respiration and transpiration of minimally processed pineapple at different storage temperatures.

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