# Modelling passive modified atmosphere packaging of strawberries: Numerical analysis and model validation

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#### <u>Article history</u>

<u>Abstract</u>

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#### <u>Keywords</u>

Respiration rate Mathematical modelling Finite element method Shelf -life Transport phenomena The aim of the present study was to develop a simple but comprehensive mathematical model for predicting molecular oxygen ( $O_2$ ), carbon dioxide ( $CO_2$ ) and temperature evolution inside modified atmosphere packages of strawberries (*Fragaria x ananassa* cv. San Andreas) during storage in fluctuating temperature conditions. Gas transport and heat transfer within packages were modelled with traditional transport phenomena approach. A combined Michaelis – Menten - Arrhenius respiration model for strawberries was included. For model validation, experimental assays with strawberries packaged in passive atmosphere and stored at different temperatures for 4 d were carried out. Simulated concentration of  $O_2$  and  $CO_2$  and temperature evolution inside packages were compared to experimental values and model adequacy was checked by calculation of Root Mean Square Error (RMSE). Implementation of model was done using COMSOL Multiphysics (version 3.4, COMSOL Inc., Burlington, MA). Results showed a good agreement between experimental data and numerical ones, at least as regards mass transfer. Less adherent experimental evidence was the prediction of temperature during the process. Model can be used to test different package configurations in order to achieve adequate postharvest storage conditions for shelf – life extension of strawberries.

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# Introduction

Modified atmosphere packaging (MAP) and low temperature storage are one of the most employed techniques to preserve freshness and safety of minimally processed fruit and vegetable products (Ragaert et al., 2004; Sandhya, 2009). MAP technology consists in package interior atmosphere modification by the interplay between product respiration, film permeability and temperature variation during storage (Mangaraj et al., 2009). Inside packages,  $\boldsymbol{\mathrm{O}}_{\! 2}$  concentration is reduced while CO<sub>2</sub> concentration increases, causing a reduction in product's respiration rate and a consequent slowing down of senescence and decay phenomena (Das et al., 2006). MAP technology finds acceptance from manufacturers because they can sell food products that stay fresh longer than products kept in atmospheric composition (Velu et al., 2013).

MAP technology requires careful design in order to result in shelf–life extension and quality retention. Excessive  $O_2$  depletion and  $CO_2$  production, for example, can lead to rapid quality deterioration and may pose risks to product safety. In particular, temperature fluctuations during storage and handling can result in important deviations from favourable atmospheres. Tano *et al.* (2008) assayed fluctuating temperatures for strawberry storage and found

\*Corresponding author. Email: *sbarrios@fing.edu.uy* Tel: +59827114478 int. 103 irreversible detrimental effects on odour, firmness, infection and colour.

Mathematical modelling has appeared in the last years as a useful tool for MAP design, enabling virtual analysis of different package configurations. Mathematical modelling can allow the prediction of package performance in terms of atmospheres and temperatures developed throughout shelf – life when exposed to fluctuating temperature conditions. Recent advances in mathematical modelling and numerical methods have permitted the solution of complex systems of equations in three-dimensional geometries, reducing the number of necessary trials to study the performance of MAP designs (Rennie and Tavoularis, 2009b).

To date, few space-and-time dependant 2D and 3D models are available in literature for MAP of horticultural produce in non-perforated packaging systems. These type of models are specially important for products where local  $O_2$  and  $CO_2$  concentrations may trigger storage disorders (Lammertyn *et al.*, 2003a,b). MAP models developed until now have considered packaging of simple - shaped vegetable products. Cefola *et al.* (2005) modelled transport phenomena occurring in a 2D MAP configuration of Cardoncello mushroom, developing what they called a 'distributed-parameters' model. They compared  $O_2$  and  $CO_2$  concentrations throughout storage



time with those obtained experimentally and by a 'concentrated-parameter' model, which described  $O_2$  and  $CO_2$  evolution solely on a time basis. Model validation was achieved for both models tested.

De Bonis *et al.* (2013) developed a 3D model for active and passive MAP of peeled ellipsoid cactus pear and took into account both respiration and microbial growth effect's on package headspace gaseous composition evolution throughout storage time. Their model was validated for three storage scenarios including different packaging atmospheres and storage temperatures and proved to be a promising analytical tool for MAP design.

Difficulties arise in multidimensional 3D modelling when actual shape of products need to be considered, since it can be money and time-consuming and has often scarce applicability (each single product is characterized by its own shape and geometry and it is impossible to have two products that are identical). Uyar and Erdogdu (2012) discussed the importance of geometrical characterization (measurement of dimensions and estimation of surface area and volume) of an object to be considered in a model and they showed that, in some cases, produces of any shape and geometry can be modelled as spheres, by simply using the volume to surface area ratios of the produces themself. Thus, they demonstrated that - by considering the same volume to surface area ratio - it is possible to overcome the determination of actual shape and geometry of a product to be considered in a heat transfer model.

In this work, given the practical importance of MAP modelling and the need for models with high and straightforward applicability to a wide range of horticultural products and packages, the aim was to develop a space-and-time dependant mathematical model for simulating O<sub>2</sub>, CO<sub>2</sub>, and temperature exchanges in passive modified atmosphere packaging of strawberries under fluctuating temperature conditions, by considering products not with their actual shape and geometry but as a layer, characterized by a certain void degree and by a volume to surface ratio same as the one of all produces included in the package. Thus, a simple but effective model is presented as a proposal of virtual laboratory useful to apply the advantages of mathematical modelling in the field of design and optimization of modified atmosphere packaging.

# **Materials and Methods**

The general structure of the present study is described as follows: 1) a model for MAP packaging of strawberries was theoretically developed to predict

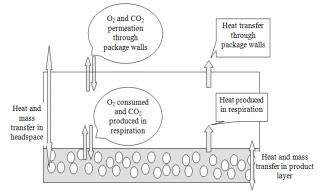


Figure 1. Schematic representation of a modified atmosphere package of strawberries. Relevant transport phenomena included in the model are summarized and allocated to corresponding sites inside package.

 $O_2$  and  $CO_2$  concentrations and temperature evolution inside packages; 2) Respiration rate modelling was performed in a previous study (Barrios *et al.*, 2014) and experimental data was included in theoretical model; 3) Model was numerically implemented using a simulation software. Simulation was run for 100 h storage time at fluctuating storage temperature conditions; 4) Strawberries were packaged and stored in fluctuating temperature conditions and  $O_2$  and  $CO_2$ concentrations and temperature evolution inside packages was experimentally determined in order to compare experimental data with simulation results and thus validate theoretical model.

# Development of a mathematical model

Development of mathematical model consisted in establishing model assumptions and mathematical description of relevant respiration and heat and mass transport phenomena occurring inside a passive modified atmosphere package of strawberries. Figure 1 presents a schematic diagram of a MA package and a summary of phenomena included in the model.

#### Model assumptions

• Commodity and headspace are isotropic.

• Only mass transport of  $O_2$  and  $CO_2$ , and heat transfer are considered as relevant transport phenomena in MAP.

- Gases behave as ideal gases.
- Commodity is modelled as product layer.
- Headspace consists of a stagnant film of air.
- CO<sub>2</sub> solubility in commodity is negligible.
- Storage temperature fluctuates according to an arbitrary variation: 2 d at 4°C, 1 d at 10 °C and 1 d at 20°C.
- Storage atmosphere composition outside package is constant and equal to air composition: 79%  $N_2$ , 21%  $O_2$ , 0.04%  $CO_2$ .
- · Initially, commodity and headspace temperatures

are uniform and equal to  $To = 15^{\circ}C$ .

• Commodity respiration follows Michaelis – Menten type kinetics.

• Variation of respiration with maturity and senescence is not considered.

• Respiration and film permeability exhibit Arrhenius temperature dependence.

#### Transport phenomena involved

For the construction of the present model, the following transport phenomena were accounted for:

1) Mass transfer of gaseous species  $O_2$  (g) and  $CO_2$  (g):

• Consumption of  $O_2(g)$  and formation of  $CO_2(g)$  at product layer

• Simple diffusion of species in product and headspace

• Permeability of gaseous species (O<sub>2</sub>, CO<sub>2</sub>) through package walls

2) Heat transfer in commodity and headspace:

• Heat production due to respiration in product (Q<sub>r</sub>)

• Heat conduction in product and headspace

• Heat transfer between package walls and surrounding atmosphere

#### Respiration modelling

Respiration involves the oxidation of energyrich organic substrates normally present in cells to simpler molecules ( $CO_2$  and  $H_2O$ ) with the concurrent production of energy (ATP and heat) (Robertson, 2006). Aerobic respiration yields the highest amount of energy, and its overall equation can be written as follows:

 $C_6H_{12}O_6 + 6 O_2 \rightarrow 6 CO_2 + 6 H_2O + energy$ 

Respiration is highly dependant on internal commodity temperature and  $O_2$  and  $CO_2$  concentrations to which commodity is exposed (Kader and Saltveit, 2002; Robertson, 2006). Several models for  $O_2$  consumption and  $CO_2$  production due to respiratory activity consider Michaelis - Menten type equations (Lee *et al.*, 1991; Peppelenbos and van't Leven, 1996). Respiration was modelled in this work according to the following equations:

$$RR_{O2} = \frac{vm_{O2} c_{O2}}{km_{O2} + c_{O2}}$$
(1)

$$RR_{CO2} = RQ \cdot RR_{O2} \qquad (2)$$

where  $vm_{02}$ ,  $km_{02}$  and RQ are, respectively, the maximum O<sub>2</sub> consumption rate, Michaelis - Menten

Table 1. Parameter values for respiration rate model of San Andreas strawberries (Barrios *et al.*, 2014)

Parameter	Value
А	1.6E13 ml kg <sup>-1</sup> h <sup>-1</sup>
Ea	64200 Jmol <sup>-1</sup>
km <sub>O2</sub>	1.9%
RQ	0.8

constant for  $O_2$  consumption and Respiration Quotient. Temperature dependence of respiration was included in the model by modelling the variation in the maximum  $O_2$  consumption rate with an Arrheniustype equation (Hertog *et al.*, 1998):

$$vm_{O2} = A \exp\left(\frac{-Ea}{RT}\right)$$
 (3)

In these equations, A is a pre-exponential factor corresponding to respiration rate when temperature tends to  $\infty$ , Ea is the activation energy associated with respiration process, R the ideal gas constant and T commodity temperature.

Respiration rate parameters included in Equations 1 and 3 were determined by non-linear regression of respiration rate data obtained by respiration rate measurements, as explained in a previously published paper (Barrios *et al.*, 2014). RQ values were determined experimentally in the cited paper. Table 1 presents parameter values for respiration rate model considered in this study.

Mass transport in product layer and in package headspace

Transport of  $O_2$  and  $CO_2$  in commodity layer and headspace was modelled using a traditional Transport Phenomena approach, considering simple diffusion of species as the only relevant transport mechanism. Convection was assumed to be negligible because headspace air was considered stagnant. By using equations of continuity for mass transport (Bird *et al.*, 2002), concentration profiles can be determined at all positions inside package throughout storage time. At commodity:

$$\frac{\partial c_{o2}}{\partial t} + \nabla \cdot (-D_{o2} \nabla c_{o2}) = -\frac{v m_{o2} \cdot c_{o2}}{k m_{o2} + c_{o2}} \qquad (4)$$
$$\frac{\partial c_{co2}}{\partial t} + \nabla \cdot (-D_{co2} \nabla c_{co2}) = RQ \cdot \frac{v m_{o2} \cdot c_{o2}}{k m_{o2} + c_{o2}} \qquad (5)$$

At headspace:

$$\frac{\partial c_{O2}}{\partial t} + \nabla \cdot (-D_{O2\_air} \nabla c_{O2}) = 0 \quad (6)$$

$$\frac{\partial c_{CO2}}{\partial t} + \nabla \cdot (-D_{CO2\_air} \nabla c_{CO2}) = 0 \quad (7)$$

In these equations, *D* stands for diffusivity of species both in commodity matrix and in headspace

air. Data for diffusivity of species in product matrix and in air was obtained from specific references (Lammertyn *et al.*, 2003a; Saravacos, 2005; Green and Perry, 2008).

#### Mass transport at and through package walls

 $O_2$  and  $CO_2$  will permeate in and out of package according to their specific permeabilities and local temperature. To model mass transfer of these species though package walls, we assumed that a convective mass transfer mechanism governs the process. Therefore, flux of gaseous  $O_2$  and  $CO_2$  was modelled according to the following equations:

$$N_{O2} = kc_{O2}(c_{O2} - cb_{O2})$$
(8)  
$$N_{CO2} = kc_{CO2}(c_{CO2} - cb_{CO2})$$
(9)

where N corresponds to a flux per unit area of package wall, kc represents mass transfer coefficient at package surface and cb stands for bulk concentration in surrounding storage atmosphere. For calculation of kc, we incorporated package permeability for each specific gas and its dependence on temperature according to an Arrhenius-type equation. Equations 10 and 11 show the relationships proposed to model mass transfer through package walls:

$$kc_{x} = P_{x} \frac{1}{86400} 1E - 6$$
(10)  
$$P_{x} = P_{x,ref} \exp\left(\frac{Eap_{x}}{R} \left(\frac{1}{T_{ref}} - \frac{1}{T}\right)\right)$$
(11)

In these equations, the subscript X represents  $O_2$  or  $CO_2$ , P represents package permeability for each of the species, T is the local temperature,  $P_{ref}$  is package permeability at a reference temperature  $T_{ref}$  and  $Ea_p$  accounts for activation energy associated with permeation process. Mass transfer coefficient  $k_c$  was derived from steady-state permeation theory or solution – diffusion model, which describes the permeation process as a coupled dissolution and diffusion process, where gaseous species first dissolve and then diffuse due to concentration gradients across the packaging film (Robertson, 2006). Numerical constants in Equation 10 are appropriate unit conversion factors. Arrhenius constants for Equation 11 were derived from Mangaraj *et al.* (2009).

# Heat production due to respiration

Respiration is a metabolic process which produces energy for cell functioning. The amount of energy produced depends on the substrate being consumed (Rennie and Tavoularis, 2009a). Modelling work of Song *et al.* (2002) included an equation for heat flux produced in respiration, which we incorporated in the present model as follows:

$$Q_r = \left(\frac{2816}{6}\right) \left(\frac{RR_{O2} + RR_{CO2}}{2}\right)$$
 (12)

This equation considers that 2816 kJ are produced for every mol of substrate consumed and that product respiration rate is the average between  $O_2$  consumption and  $CO_2$  production rates. An average respiration rate is considered in order to take into account the variability of respiration quotients with the nature of the respiration substrate (glucose, organic acids, etc.).

# Heat transfer in product layer and at package headspace

Respiratory energy dissipated as heat is transported by conduction mechanism in product layer and in package headspace. No transport by convection was considered in our work because headspace air was considered stagnant. A traditional Transport Phenomena approach was also used to model heat transfer, applying energy equation of change (Equation 13; Bird, Stewart and Lightfoot, 2002):

At commodity:

$$\rho C_{p} \frac{\partial T}{\partial t} - \nabla \cdot (k \nabla T) = Q_{r} \quad (13)$$

At headspace:

$$\rho_{air}C_{p_{air}}\frac{\partial T}{\partial t} - \nabla \cdot (k_{air}\nabla T) = 0 \qquad (14)$$

By solving these equations in product layer and in package headspace, a temperature profile can be obtained throughout storage time. Physical properties  $\rho$ , Cp and k for product and headspace air were obtained from specific references (Nesvabda, 2005; Green and Perry, 2008).

#### Heat transfer at and through package walls

To model heat transfer across package walls, we considered a convective mechanism according to the following heat flux:

$$Q_p = h_p \left( T - T_{ext} \right) \qquad (15)$$

where  $Q_p$  is the heat flux per unit area of package,  $h_p$  is the convective heat transfer coefficient and  $T_{ext}$  is the external surrounding ambient temperature. To calculate  $h_p$ , the model proposed by Song *et al.* (2002), based on the work by Toledo (1991), was considered:

$$h_{p} = 3600 \left[ \frac{0.59 A_{p1} \left| \frac{T - Text}{D_{1}} \right|^{0.25}}{A_{p}} + \frac{1.32 \cdot A_{p2} \left| \frac{T - Text}{D_{2}} \right|^{0.25}}{A_{p}} + \frac{1.42 A_{p3} \left| \frac{T - Text}{D_{3}} \right|^{0.25}}{A_{p}} \right]$$
(16)

This heat transfer coefficient is derived from a correlation which considers the top of the package as a horizontal small plate facing upwards when cooled, the bottom of the package as a horizontal small plate facing downwards when cooled, and the sides of the package as vertical small plates (Song *et al.*, 2002).

# Determination of commodity layer height and volume

Commodity was modelled as a layer of fruit, characterized by a certain void degree and by a volume to surface ratio same as the one of all produces included in the package, without considering actual geometry of bed of strawberries. In order to maintain the actual strawberry mass packaged in trays, volume of strawberry layer was determined by considering a certain void volume that lowered strawberry layer's bulk density ( $\rho_{bulk} = 600 \text{ kgm}^{-3}$ ; Zanderighi, 2001). Actual mass of strawberries packaged and bulk density determined a certain layer volume, and thus a layer height, which better represented surface area/headspace volume relationship while maintaining actual strawberry mass packaged in trays.

# Initial conditions

Initial conditions for commodity, headspace and ambient atmosphere composition were that of air:  $21\% O_2$  and  $0.04\% CO_2$ . Initial external temperature was uniform and equal to 8°C. Initial commodity and headspace temperatures were uniform and set at 15°C according to experimental data.

### Model solution

Mathematical model developed was implemented using COMSOL Multiphysics (version 3.4, COMSOL Inc, Burlington, MA), a software package which solves partial differential equations using the Finite Element Method. Computational domain consisted in two subdomains: commodity and headspace. Equations were assigned to their corresponding subdomains and solved using second-order Lagrange elements. Transport phenomena occurring at interfaces (commodity - headspace and headspace packaging film) were assigned to boundary conditions. Meshing was done with tetrahedral elements and required grid independence studies were carried out by comparing solutions achieved using three different mesh densities (Romano and Marra, 2008; Rennie and Tavoularis, 2009b). Meshing was done with 56411 tetrahedral elements and 245346 degrees

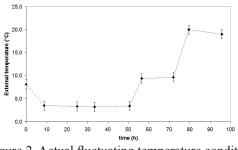


Figure 2. Actual fluctuating temperature conditions imposed on stored strawberries

of freedom. The GMRES iterative solver was used with a geometric multigrid preconditioner. Relative and absolute tolerances were set at 0.1 and 0.01 respectively.

Computations were conducted on a personal computer with a 1.6 GHz Intel Pentium Dual CPU and 960 MB RAM under Microsoft Windows XP Professional. Typical solution times ranged from 9 to 9.6 hours.

# Model validation

Numerical implementation of mathematical model was tested by comparing model predictions with experimental data obtained for  $O_2$ ,  $CO_2$  and headspace temperature evolution monitoring inside strawberry packages.

Strawberries (*Fragaria* x *ananassa* cv. San Andreas) were obtained from a local producer near Montevideo (Uruguay). Fruits were harvested at commercial maturity stage and transported under ambient conditions to Facultad de Ingeniería (Montevideo, Uruguay) within 12 hours. Upon arrival at the laboratory, strawberries were qualitatively selected based on colour, size, and absence of defects to obtain a homogeneous batch.

Strawberries  $(200 \pm 10 \text{ g})$  were selected at random and placed in polyestyrene trays under normal air. Trays were packaged using 20 x 30 cm low density polyethylene (PE) bags (30 µm thickness) of known transmission rates ( $P_{02} = 5100 \text{ cm}^3 \text{ m}^{-2} \text{ d}^{-1}$  at 23°C;  $P_{C02} = 16000 \text{ cm}^3 \text{ m}^{-2} \text{ d}^{-1}$  at 23°C). Arrhenius constants for PE film were obtained from data presented by Mangaraj et al. (2009). Bags were filled with air and heat - sealed using a Supervac GK105/1 packaging machine (Wien, Austria). Strawberries were stored in temperature fluctuating conditions for 4 d with the following temperature variations: 2 d at 4 +/- 1 °C, 1 d at 10 +/- 1 °C and 1 d at 20 +/- 1°C (Figure 2). Relative humidity inside storage chamber was 80 -85%. O<sub>2</sub> and CO<sub>2</sub> concentrations and temperature inside packages were evaluated in triplicate two times a day and separate replicate bags were assessed at each sampling point. O<sub>2</sub> and CO<sub>2</sub> concentrations

inside packages were determined by extracting a 15 mL gas sample directly from the package through a needle and a silicon tube and analyzing it using a Servomex 1450C Food Package Analyzer (Crowborough, Sussex, UK). The whole packaging trial was repeated three times with a different batch of strawberries for result verification.

Differences between simulated (simul) and experimental (exp) results for  $O_2$ ,  $CO_2$ , and headspace temperature, for the n sampling points, were evaluated by means of Root Mean Square Error (RMSE), calculated by the following equation (Yang and Chinnan, 1988):

$$RMSE = \sqrt{\frac{\sum_{i=1}^{n} \left[ (\exp)_{i} - (simul)_{i} \right]^{2}}{n}} \qquad (17)$$

RMSE values lower than or close to 2 validate adequacy of the model.

# **Results and Discussion**

# Headspace O<sub>2</sub> and CO<sub>2</sub> composition evolution

Figure 3 shows experimental and simulation results for concentration of O<sub>2</sub> and of CO<sub>2</sub> evolution in the headspace throughout 100 h storage. Experimental and simulated O<sub>2</sub> and CO<sub>2</sub> evolution curves showed three different zones with different consumption and production rates, in response to the three temperature zones identified in Figure 2. Temperature has a major effect on produce respiration rate (Robertson, 2006), and this effect is generally higher that temperature effect on packaging film permeability. Therefore, as temperature increased, the change in headspace composition due to respiration rate is more important than the gas migration through the permeable packaging film, resulting in modified atmospheres in terms of O<sub>2</sub> and CO<sub>2</sub> composition. More in detail, temperature increases resulted in reduced O2 and increased CO, compositions, because the higher the storage temperature, the higher the consumption and production rates of O<sub>2</sub> and CO<sub>2</sub> respectively. Strawberries are highly respiring produce (Li and Kader, 1989), so significant modifications in headspace composition were expected, specially at 10 and 20°C. From Figure 3 it can be seen that  $O_2$  and CO<sub>2</sub> concentrations had significantly changed within 2 d storage at 4°C ( $O_2 = 15\%$  and  $CO_2 = 5\%$ ). Changes in headspace atmosphere were enhanced in these first hours of storage by the fact that strawberry's initial temperature was  $To = 15^{\circ}C$ , so strawberries were exposed to temperatures over 4°C for almost 10 h (Figure 4). By the end of storage, temperature effects on respiration rate were so significant that anaerobic conditions were reached inside packages and CO<sub>2</sub> had

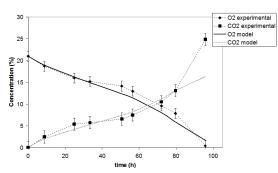
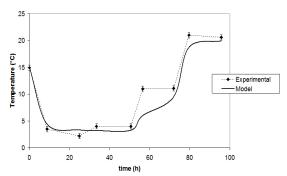
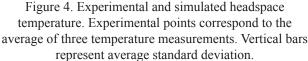


Figure 3. Experimental and simulated  $O_2$  and  $CO_2$  evolution. Experimental points correspond to the average of three measurements. Vertical bars represent average standard deviation.





built up to 25%. Anaerobic conditions are undesirable for packaging of horticultural products (Robertson, 2006), so temperature abuse such as the one exercised in this paper should be avoided.

RMSE values of 1.2 and 2.9 were obtained for O<sub>2</sub> and CO<sub>2</sub> model curves respectively, indicating that O<sub>2</sub> simulation adequately fit experimental data, yet CO<sub>2</sub> evolution fit was not as good. Examination of Figure 3 shows that high RMSE value for CO<sub>2</sub> evolution was probably due to the difference between simulated and experimental values only at 96 h storage. Model could not predict the sudden increase in CO<sub>2</sub> concentration registered from 80 to 96 h storage. A possible explanation for this sudden increase is that exposure to 20°C from 80 to 96 h storage could have caused physiological responses or accentuated microbial growth and this may have led to an increased CO<sub>2</sub> production. This explanation seem more plausible if one examines Figure 4, where it is clear that temperature did increase in a sudden manner from 10°C to 20°C, so temperature effect was effectively reflected on O<sub>2</sub> and CO<sub>2</sub> evolution. De Bonis et al. (2013) modelled mesophilic and psychrotropic bacteria development in MAP at 8°C and concluded that significant growth was verified at this temperature. Models that take into consideration respiration of microorganisms, in addition to product respiration, could be important in cases were temperature abuse determines significant microbial growth.

As for  $O_2$  concentrations,  $O_2$  evolution falls out of interval defined by standard deviation between 50 and 80 h storage, coinciding with the period where temperature evolution showed its less adequate fit (see below). In the period 80 to 96 h, acceleration in  $O_2$  consumption was verified and model predicted final  $O_2$  concentrations relatively well. Highest deviations from experimental data were of 25% for this variable.

#### *Headspace temperature*

Experimental and simulation results for headspace temperature are shown in Figure 4. An RMSE value equal to 2 was calculated for this variable. Although this RMSE value indicated an adequate model fit to experimental data, some aspects of Figure 4 are to be remarked. As expected, three temperature zones were clearly distinguished: the initial lowering and maintenance of temperature at 4°C, the increase to 10°C and the increase to 20°C. However, simulation showed inertia to temperature changes, specially when increasing temperature, that experimental evolution did not. At 56 h, for example, simulation could not rise headspace temperature as fast as was verified in experimental runs. In fact, simulated temperature is always rising from 4 to 10°C, while experimental temperature evolution showed that there was a constant temperature period after reaching 10°C and until 72 h storage. Something similar happened with the rise from 10 to 20°C at 80 h storage, although in this case inertia was reduced and model fit to experimental data was better.

Another aspect to be highlighted is that, regardless of RMSE value, simulated temperature evolution did not fall within the interval defined by experimental temperature standard deviation. This could be showing that heat transfer equations included in theoretical model within MA strawberry package were insufficient to account for heat transfer phenomena. Inclusion of convective heat transfer as a transport mechanism should be tested in further simulations for this package configuration.

Incomplete fitting of modelling results with experimental data, both for  $O_2$  and  $CO_2$  evolution, could also be related to the geometrical approximation exercised for implementation of the present model. Even though approximation of a strawberry bed with a simple layer seems rather radical, authors believe that differences between one approach and another are considerable in the case of higher layer heights, were internal heat and mass transfer would impose

Nomenclature Mass flow (mol m² s·ľ Arrhenius pre-exponential factor (ml kg1 h A. Total package surface area (m2) Packaging film permeability (cm3 m 2 d-1) Pref Packaging film permeability at reference temperature (cm3 m 2 d-1) Top package surface area (m2) Bottom package surface area (m2) Q, Respiratory heat (W m3) Heat flux at package surface (J s-1 m2) A Side package surface area (m2) Q, Ideal gas constant (8.314 J mol-1 K-1) Concentration (mol m3 or %) c cb Ambient concentration (mol m3) RO Respiration Quotient Specific heat (J kg1 K-1) RR Respiration rate (ml kg-1 h1) Diffusivity (m<sup>2</sup> s Surface area (m2) S Top package length (m) Temperature (K) Bottom package length (m) Text External temperature (K) Side package length (m) To Initial temperature (K) Activation energy (J mol<sup>1</sup>) Tref Reference temperature (K) Eap Permeability activation energy (J mol-1 ) time (s) Heat transfer coefficient at package surface (J s-1 m-2 K-1) V Volume (m3) Thermal conductivity (I s1 m1 K-1) Maximum respiration rate (ml kg-1 h1) vm<sub>o2</sub> Mass transfer coefficient (m s-1) Density (kg m3) kc Michaelis - Menten constant (%) km<sub>o</sub> Subscripts Oxygen  $0_{2}$ CO<sub>2</sub> Carbon Dioxide Δir

higher gradients. In the case considered in this study, differences between a strawberry bed approach and a layer approach should be reflected, reasonably, in the relatively small discrepancies observed for  $O_2$ ,  $CO_2$  and temperature evolution throughout most of the storage time.

# Conclusions

The main transport phenomena of energy and mass involved in respiration of strawberries packed in modified atmosphere were simulated by means of resolution of a mathematical model, in which geometric simplification has allowed to overcome the difficulties linked to the inevitable difference in shape and size that any fruit has. Goodness of results of numerical analysis was evaluated by comparison with experimental observations, both in terms of evolution of oxygen and carbon dioxide concentration, and in terms of temperature evolution in the headspace of the package. Results showed a good agreement between experimental data and numerical ones, at least as regards mass transfer. Less adherent experimental evidence was the prediction of temperature during the process. Reliability of this approach is to be considered good and intuition concerning the simplification of the geometric representation of whole fruits' volume appears to be very promising. Certainly there is room for improvement, especially in the formulation of the energy balance, which will be subject to further investigations and future developments.

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