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A comprehensive simulation program for modified atmosphere and humidity packaging (MAHP) of fresh fruits and vegetables

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ABSTRACT

Modified atmosphere and humidity packaging (MAHP) is used to extend shelf life and maintaining the quality of fresh fruits and vegetables by modifying desired gas concentration and relative humidity (RH) inside fresh produce package. Several factors affect the optimum design of MAHP, most of which are time and or temperature dependent. Hence, there is a vital need for a simulation tool that includes all affecting parameters and their interactive behavior on package gas composition and water vapour. In this study a comprehensive simulation program based on integrative mathematical modeling is presented. A number of validation experiments were conducted to evaluate the robustness of the simulation program under constant and varying temperature conditions during storage period and predict gas composition, humidity and moisture condensation dynamics in packaged strawberry and plum. The simulated results were satisfactory with those obtained experimentally. The validated simulation program was then used for optimization of modified humidity packaging for both plum and strawberry. The predicted equilibrium headspace humidity was 94.0 and 98.8% for strawberries and plums, respectively which was very close to measured values of 93.5 and 94.1%, respectively. Therefore, the simulation program was found to be a convenient tool to virtually test the package under a broad range of environmental conditions such as temperature and RH resembling real supply chain conditions and ensure proper selection of packaging systems for the optimum performance.

1. Introduction

Several factors affect post-harvest quality of fresh produce. Amongst them, some biological phenomena such as respiration and transpiration are of great importance. Respiration is a metabolic process that provides energy for plant biochemical processes (Fonseca et al., 2002). One important consequence of respiration on fresh produce quality is weight loss of produce, due to oxidative breakdown of substrate molecules such as starch, sugars, and organic acids to simpler molecules such as CO_2 and H_2O. This process generates some heat as well, major part of which leaves produce surface by evaporating water vapour from surface layers (Kader and Saltveit, 2003). Also fruits continuously lose water to the atmosphere by transpiration since ambient atmosphere normally has a much lower water potential than produce surface (Rodov et al., 2010). Water loss is one of the main causes of commercial and physiological deterioration of fresh produce, in the form of wilting, shriveling, and decrease of stiffness, turgidity and succulence (Rodov et al., 2010).

Modified atmosphere packaging is an active or passive dynamic process of modifying gaseous composition within a package. Passive approach just relies on natural initial gaseous composition as well as the interaction between the respiration rate of the produce, and the permeation of gases through the packaging material especially packaging film, while in active approach, gases of desired composition are additionally flushed into the package in order to achieve faster equilibrium atmosphere (Caleb et al., 2012; Farber et al., 2003; Mahajan et al., 2007). However, improper control of respiration may lead to undesirable results from low level of O_2 and consequently anaerobic respiration, accelerated physiological decay, and shortened shelf life (Song et al., 2002). Resistance of a plastic film for water vapour permeation usually far exceeds that of produce surfaces. Therefore, most water molecules evaporated from the produce do not escape through the film and remain within the package space, enhancing the water vapour pressure in the package headspace and or condense on fruit and tray wall surfaces,

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which accelerates spoilage and considerably shortens storage life (Ben-Yehoshua et al., 1998; Kleinhenz et al., 2000; Rodov et al., 2010; Xu and Burfoot, 1999). Hence, modified atmosphere and humidity packaging (MAHP) is used to modify package humidity in addition to gas composition, in order to control the amount of transpiration by decreasing water potential difference and hence preventing water loss (Ben-Yehoshua et al., 1996; Morris and Jobling, 2000; Rodov et al., 2003).

There have been few studies on relative humidity (RH) and condensation in modified atmosphere packaging of fruits and vegetables. Song (1995) presented a mathematical modeling approach based on heat and mass transfer for respiration and transpiration behavior to predict RH in MAP of fresh produce. They could successfully validate the model for blueberry and stated that RH can't be controlled well below 100% using commercial packaging films they used. Song et al. (2001) later modified the model presented by Song (1995) based on respiratory and transpiratory behavior of the fresh produce, the transport phenomena across the package, and the moisture sorption behavior of two commercially available moisture absorbent. Although model predictions agreed well with experimental results, but no further attempts were made to determine the amount of condensation. This can be due to the fact that model predictions showed that the temperature variation was not significant at fruit surface and hence no condensation occurred. Lu et al. (2013) presented a model based on heat and mass transfer for predicting RH within the package. Except for initial period, their model agreed well with experimental data. The package headspace was chosen small; therefore, they neglected the needed time to achieve thermal equilibrium and accordingly condensation occurrence. In contrast, Linke and Geyer (2013) identified the intensity and retention time of condensation on fruit surface, internal film and tray wall surfaces as main determinant of condensation dynamics in fresh produce packaging under fluctuating ambient temperature. However, only experimental approach was used to measure the condensation formation under varying experimental conditions while suggesting mathematical modeling as a future scope. Mathematical modeling approach needs several factors and parameters for simulating condensation dynamics (Table 1), most of which are time and or temperature dependent. Hence the aim of this study was to develop a simulation tool based on integrative mathematical modeling to predict the packaging headspace gas composition and relative humidity (RH), as well as condensation dynamics in fresh produce package headspace. Such a simulation tool was then applied for packaging design for strawberries and plums under varying environmental conditions such as temperature and relative humidity, resembling realistic conditions in fruit supply chain.

2. Model development

2.1. Rate of moisture loss from product

Fresh produce continues to lose moisture after harvest due to both transpiration and respiration (Bovi et al., 2016). Aerobic respiration (i.e., biological oxidation) is the oxidative breakdown of complex substrate molecules such as starch, sugars, and organic acids-to simpler molecules such as carbon dioxide and water and regeneration of ATP from ADP (adenosine diphosphate) and Pi (inorganic phosphate). If hexose sugar like glucose coming from stored simple sugars (e.g., glucose, sucrose) or complex polysaccharides (e.g., starch), is used as the substrate, the overall equation can be written as Eq. (1):

$$C_6H_{12}O_6 + 6\,O_2 + 38\,ADP + 38\,Pi \rightarrow 6\,CO_2 + 6\,H_2O + 38\,ATP + 2816\,kJ \tag{1}$$

For respiratory oxidation of 180 g (1 mol) of glucose, 192 g (6 mol) of O_2 is consumed which diffuses into the tissue from surrounding atmosphere, while 264 g (6 mol) of CO_2 diffuses out. The 108 g (6 mol) of H_2O produced is simply incorporated into the aqueous solution of the cell. From the 2816 kJ that is capable of doing work, around 1176 kJ (41%) is used to produce 38 ATP molecules (38 ATP × 30.96 kJ/ATP) and remaining 1640 kJ (57%) is lost as heat (Kader and Saltveit, 2003). If all of the heat produced leaves the tissue by vaporizing water, the rate of moisture loss due to respiration can be related to produce respiration rate as shown in Eq. (2).

$$\frac{dM_{rr}}{dt} = \frac{R_{CO2}\,W_p}{264} \times \frac{1640}{H_v} = \frac{R_{CO2}\,W_p\,(1640/264)}{\left(-6.14\times10^{-5}T^3 + 1.58\times10^{-3}T^2 - 2.36T + 2500.7\right)\times10^{-3}} \tag{2}$$

where the dominator of right hand fraction is equal to H_v as a function of temperature (Yau and Rogers, 1996). Total weight loss is the sum of moisture loss by respiration heat, carbon loss from substrate oxidation minus water produced in respiration reaction

Table 1
Variables affecting design of modified atmosphere and modified humidity packaging for fresh fruit and vegetables.

Fresh produce:
- Physiological properties (respiration and transpiration rate models, water activity)
- Physical properties (weight, density, volume, surface area, geometrical shape)
- Thermal properties (specific heat, thermal conductivity and diffusivity, surface convective heat and mass transfer coefficient)

Package system:
- Physical properties of tray (weight, volume, surface area, geometrical shape)
- Physical properties of lidding film (thickness, surface area, permeability to gases and water vapour, micro and macro-perforations)
- Physical properties of humidity absorbers (absorption kinetic models)
- Thermal properties of packaging materials (specific heat, thermal conductivity and diffusivity, surface convective heat transfer coefficient)

Ambient storage conditions:
- Temperature and relative humidity of air surrounding the package
- Gas composition (O_2 and CO_2)
- Air flow speed around the package

remaining in the fruit texture.

Fruit respiration leads to decrease in O_2 and increase in CO_2 level within the package. Data reported by Saltveit et al. (2004) as well as Michaelis-Menten type models (Eqs. (3) and (4)) reported by Hertog et al. (1999) were used to estimate R_{O_2} and as R_{CO_2} which are needed in Eqs. (2), (12) and (13).

$$R_{O_2} = \frac{O_2^{in}}{K_{mO_2} + O_2^{in}} Vm_{O_2}^{ref}\, e^{\frac{E_{aO_2}}{R}\left[\frac{1}{T_{ref}} - \frac{1}{T_i}\right]} \tag{3}$$

$$R_{CO_2} = RQ_{ox}\, R_{O_2} + \frac{1}{\left(1 + \frac{O_2^{in}}{K_{mCO_2(f)}}\right) + 1} Vm_{CO_2(f)}^{ref}\, e^{\frac{E_{aCO_2(f)}}{R}\left[\frac{1}{T_{ref}} - \frac{1}{T_i}\right]} \tag{4}$$

2.2. Rate of gas and water vapour transfer through packaging film

As common plastic films used in MAP are not enough permeable to gases and especially to water vapour, making perforations in such films can modify its permeability. One approach is using micro-perforations in packaging films. Techavises and Hikida (2008) developed a mathematical model based on Fick's law of diffusion to determine the rate of gas and water vapour permeation trough a perforated packaging film, combining the effects of film permeability and apparent permeability of micro-perforations of packaging film. Eqs. (5)–(7) are used to determine the permeation rates of O_2, CO_2 and H_2O trough packaging film respectively.

$$\frac{dP_{O_2}}{dt} = \left[N_p\, P_{eff} + \frac{K_{O_2}\, A}{e}\right] P_{atm}\left(O_2^{out} - O_2^{in}\right) \tag{5}$$

$$\frac{dP_{CO_2}}{dt} = \left[N_p\, P_{eff} + \frac{K_{CO_2}\, A}{e}\right] P_{atm}\left(CO_2^{out} - CO_2^{in}\right) \tag{6}$$

$$\frac{dP_{H_2O}}{dt} = \left[N_p\, P_{eff} + \frac{K_{H_2O}\, A}{e}\right] (P_{in} - P_{out}) \tag{7}$$

where K_i, the permeability coefficient of film to gas (i: O_2, CO_2 or H_2O) is related the transmission of gas through the polymeric film by film thickness (e) and pressure difference across it (Mangaraj et al., 2009). Also the effective permeability (P_{eff}) was independent of gases as well as temperature (Techavises and Hikida, 2008), and partial pressures of water vapour for headspace (P_{in}) and ambient (P_{out}) are given in Eqs. (8)–(10):

$$P_{eff} = \left(0.0298\, dp^2 + 0.537\, dp + 0.822\right) \times 10^{-3} \times \rho_{wv} \tag{8}$$

$$P_{in} = P_{sat} \times \frac{RH_{in}}{100} \tag{9}$$

$$P_{out} = P_{sat} \times \frac{RH_{out}}{100} \tag{10}$$

And P_{sat} is headspace partial pressure of water vapour at saturation, and is generally related to temperature according to Eq. (11) which is commonly known as the Magnus formula (Lawrence, 2005):

$$P_{sat} = C_1 exp\left[\frac{A_1 T}{B_1 + T}\right] \tag{11}$$

Alduchov and Eskridge (1996) evaluated this expression and recommend the values for the coefficients of A_1, B_1 and C_1 which provide values for partial pressure of water vapour at saturation, with a relative error of <0.4% over the range $-40\ ^\circ C \le T \le 50\ ^\circ C$.

2.3. Rate of gas changes in the headspace

The rate of O_2 consumption and CO_2 production affects concentration of relevant gases. Also the concentration of each gas depends on the gas permeation rate through packaging film. Hence, Eqs. (12) and (13) are used to calculate the rate of mass change of O_2 and CO_2 in the package headspace.

$$\frac{dMO_2^{in}}{dt} = \frac{dP_{O_2}}{dt} - R_{O_2} W_p \tag{12}$$

$$\frac{dMCO_2^{in}}{dt} = \frac{dP_{CO_2}}{dt} + R_{CO_2} W_p \tag{13}$$

2.4. Internal relative humidity and condensation

The rate of total moisture change in the packaging headspace is the sum of water vapour permeation rate through the packaging film and the rate of moisture loss due to product respiration as given in Eq. (14):

$$\frac{dM_{H_2O}}{dt} = \frac{dP_{H_2O}}{dt} + \frac{dM_{rr}}{dt} \tag{14}$$

Maximum capacity of headspace air to hold water vapour corresponds saturated vapour pressure, which is the maximum that can exist at a given temperature (Ashrae, 1997), which can be calculated using Eq. (15).

$$MH_2O_{max} = W_a \times \left[\frac{0.622 \times P_{sat}}{P_{atm} - P_{sat}}\right] \times 10^6 \tag{15}$$

where W_a is weight of dry air and is related to air density (Eq. (16)):

$$W_a = V_f \times \rho_{air} \tag{16}$$

And dry air density which varies with temperature can be calculated using Eq. (17) (Ashrae, 1997):

$$\rho_{air} = \frac{P_{atm}}{287.05\,(T_i + 273.15)} \tag{17}$$

Excess fruit moisture loss beyond MH_2O_{max}, will condense out as dew or frost (Ben-Yehoshua and Rodov, 2003; Tano et al., 2007), Therefore, the amount of condensation can be calculated as the difference between total moisture in packaging headspace and moisture content of headspace air at saturation (Eq. (18)):

$$M_{cond} = M_{H_2O} - MH_2O_{max} \tag{18}$$

And the moisture content of headspace air can be calculated by Eq. (19) as the difference between total moisture in the packaging headspace and total condensation.

$$MH_2O_{air} = M_{H_2O} - M_{cond} \tag{19}$$

When there is no condensation in the packaging headspace, all the headspace moisture is present in the headspace air.

RH_{in} was calculated from the humidity mixing ratio (H_{in}) of air (also referred as moisture ratio or specific humidity in the literature), i.e. mass of water vapour in unit mass of dry air (Ashrae, 1997), itself depending on the MH_2O_{air} coming from integration of Eq. (14):

$$H_{in} = \frac{MH_2O_{air} \times 10^{-3}}{W_{air}} \tag{20}$$

P_{in} can be calculated based on H_{in} as well (Ashrae, 1997) and also Eq. (9) was rearranged to represent RH_{in}:

$$P_{in} = \frac{P_{atm}\, H_{in}}{0.622 + H_{in}} \tag{21}$$

$$RH_{in} = \frac{P_{in}}{P_{sat}} \times 100 \tag{22}$$

Combining Eq. (20)–(22), RH_{in} can be calculated based on MH_2O_{air}:

$$RH_{in} = 100 \times \frac{P_{atm} \times \frac{MH_2O_{air} \times 10^{-3}}{W_{air}}}{P_{sat}\left(0.622 + \frac{MH_2O_{air} \times 10^{-3}}{W_{air}}\right)} \tag{23}$$

The initial value for RH_{in} is known from the experimental data and is equal to ambient RH at initial time.

2.5. Rate of fruit surface, tray wall and headspace air temperature change

Temperature change within the package affects phenomena which determine the headspace humidity and gas composition, as well as condensation. Hence all package components (headspace air, fruit surface, tray wall) transient temperature need to be predicted depending on ambient conditions varying with time. Eqs. (24)–(26) are modified form of energy balance equations (Song et al., 2002), to model the rate of temperature change for each package component.

$$\frac{dT_t}{dt} = \frac{K_t A_p (T_o - T_t)/e - h_p A_p (T_i - T_t)}{W_t C_t} \tag{24}$$

where T_o is given for all times and initial values for T_i and T_t are known from the experimental data. Also the rate of temperature change for internal tray wall is simultaneously affected by conductive heat transfer within the tray wall cross section, convective heat transfer between internal tray wall and headspace air, and sensible heat absorbed by packaging tray mass due to its heat capacity.

$$\frac{dT_s}{dt} = \frac{6.21\, R_{CO_2} W_p - \frac{dm_{rr}}{dt}\lambda + h_s A_s (T_i - T_s)}{W_p C_p} \tag{25}$$

where initial values for T_s is known from the experimental data. Also the rate of temperature change for fruit surface is simultaneously affected by heat produced by fruit respiration, convective heat transfer between fruit surface and headspace air, cooling effect of moisture evaporation from fruit surface due to moisture loss and sensible heat absorbed by fruit mass due to its heat capacity. The constant 6.21 (1640/264) is equal to heat released per oxidation of one mole glucose (1640 kJ) from which 6 mol (264 g) CO_2 is generated.

$$\frac{dT_i}{dt} = \frac{h_p A_p (T_t - T_i) - h_s A_s (T_i - T_s) + \frac{dMH_2O^{in}}{dt}\lambda}{W_a C_a} \tag{26}$$

where the rate of temperature change for headspace air is simultaneously affected by convective heat transfer between fruit surface and headspace air and between internal tray wall and headspace air and heat transfer to the air by the mass transfer from fruit moisture loss as well as moisture permeation through packaging film. Assuming natural convection inside the package, total convective heat transfer coefficient of internal tray walls was estimated by Eq. (27) (Song et al., 2002):

$$h_p = 3600\left[\frac{0.59 A_{p1}\left(\frac{T_i - T_o}{D_1}\right)^{0.25}}{A_p} + \frac{1.32 A_{p2}\left(\frac{T_i - T_o}{D_2}\right)^{0.25}}{A_p} + \frac{1.42 A_{p3}\left(\frac{T_i - T_o}{D_3}\right)^{0.25}}{A_p}\right] \tag{27}$$

where D_1, D_2 and D_3 are respectively dimensions of top, side and bottom of packaging tray with a rectangular geometrical shape. Top and bottom are assumed as a horizontal small plates facing upward and downward respectively when cooled, and side is assumed as a vertical small plate. Convective heat transfer coefficient for fruit surface (h_s) was estimated using conventional heat transfer correlations in which the dimensionless numbers for natural convection are used. Dimensionless numbers typically appearing in these correlations are the Nusselt number, the Prandtl number, the Grashof number, and sometimes the Rayleigh number (Bergman and Incropera, 2011).

2.6. Computer simulation program

All variables and modeling equations mentioned in Sections 2.1–2.5 were integrated to a computer simulation program based on MATLAB software (MATLAB R2010b, MathWorks®, USA). All time dependent ordinary differential equations (ODEs) where solved numerically using Euler's method which is a first order Runge-Kutta method for numerical integration of ODEs, to predict package components like temperature, gas, relative humidity and condensation dynamics within the package headspace as a function of several input parameters (Table 1) and display the information in graphical format.

For estimation of the water vapour condensation dynamics, it was assumed that the three factors that affect the amount of condensate are the surface area, difference between the package component temperature and dew point, and lastly the thermal properties of each package component. Based on this assumption, an approach was implemented in simulation program to assign the amount of condensate on each package component. When water vapour saturation condition is dominant in a package, dew point temperature is equal to or more than headspace temperature. Decreasing the temperature of each package component below dew point temperature makes it a potential place for condensation (Joyce and Patterson, 1994; Rodov et al., 2010; Shamaila et al., 2005; Xu and Burfoot, 1999). In contrast, when the surface temperature is raised above dew point, the condensed water starts to vaporize from that surface.

3. Validation experiments

A robust reliable simulation program of MAHP must be able to make predictions even in a narrow range of variation in the results, under various experimental conditions from constant temperature and RH to varying conditions with sharp fluctuations. On the other hand, it must be flexible to adopt with various types of fresh fruits and vegetables with different physiological and physical properties and various packaging material and physical properties. Hence, two types of fruits were used; strawberry with a high respiration and moisture loss rate rather than plum with a lower respiration and moisture loss rate (Saltveit et al., 2004). Two series of validation experiments were performed under constant and varying ambient conditions regardless the recommended storage conditions. In the end, validation was performed for controlling RH and condensation in both packaged products.

3.1. Constant temperature

Simulation program was used to predict headspace O_2, CO_2 and RH under constant conditions (10 ± 0.5 °C temperature and 60% RH) for strawberry and evaluate the effect of respiration and transpiration. These predicted results were then validated experimentally. For this, a package of size 20 × 12 × 11 cm containing 199.7 ± 0.4 g of fresh strawberry (cv. Elsanta) was used. Macro-perforations of 3 mm diameter (1, 3, 7 numbers) were made with a needle in the lidding packaging film. The lidding plastic film (polypropylene, transmission rate of 19, 76 and 26 ml $m^{-2}h^{-1}$ for O_2, CO_2 and H_2O, respectively at 23 °C and 85% RH) was obtained from Innovia films (Cumbria, UK). A special clamping tool was used to fix the lidding film onto the package tray. All the packages were equipped with an air humidity sensor FHA 646R (Ahlborn, Holzkirchen, Germany) for measuring headspace temperature and RH. The sensors were 50 mm length and 5 mm diameter. The criteria for selecting the sensors were low energy input into the packaging as well as small sensor dimensions. A separate sensor was used for ambient air measurements. The fruit surface temperature was measured using an infrared sensor (AMIR 7842, Ahlborn, Holzkirchen, Germany). Gas composition (O_2 and CO_2) of package headspace was measured every day by injecting 5 ml of sample in the gas analyzer (Dansensor, Ringsted, Denmark). All data were recorded every second using a data logger (ALMEMO 2490, Ahlborn, Holzkirchen, Germany) for the entire duration of experiment (72 h).

3.2. Varying temperature

In order to investigate the robustness of simulation program, predictions were performed under varying temperature conditions of the storage environment and for a different type of product e.g. plum (CV. Angelino). These predictions were then validated experimentally using the package as specified in section 3.1 with one 3 mm macro-perforation and plum weight of 600 g. A controlled environment chamber (Hereaus Instruments, Hameln, Germany) was used to provide varying temperature profile. It was programmed to make temperature cycles between 5 and 15 °C (3 h at 5 °C, 3 h at 15 °C with 0.5 h for temperature change over each). Two separate air humidity sensors (Ahlborn, Holzkirchen, Germany) were used, one for measuring temperature and humidity of package headspace and the other for measuring temperature and humidity conditions of storage air. In addition, seven temperature sensors (EPCOS AG, Greenville, USA) having a very small head dimensions (glass-encapsulated), diameter 0.5 mm were used inside the package to measure temperature of different package components: fruit surface, tray wall, inner tray bottom, film surface and package headspace air. All experimental data was recorded (ALMEMO 2490, Ahlborn, Holzkirchen, Germany) at second interval for the entire duration of experiment (44 h).

3.3. Application of simulation program

The validated simulation program was then used to for optimization of modified humidity packaging for both plum and strawberry. It was not possible to achieve the modified atmosphere without compromising high humidity conditions, mainly because packaging film used has a very low permeability for water vapour. The target was to achieve equilibrium RH in the range of 90–95% optimum for both plum and strawberry (Saltveit et al., 2004) in a package (12 × 16 × 6 cm) under three levels of storage temperature 5, 10 and 15 °C and a constant ambient RH of 50%. From the preliminary trails, it was determined that package volume (1150 ml) was suitable to contain 450 g of product, with a marginal variation of ±50 g. Therefore, simulations were performed at three levels of fruit weight (400, 450 and 500 g), and different numbers of perforation (in the range of 1–10 for plums and 10 to 40 for strawberry). From these simulations, optimum level of fruit weight (400 g for plum and 450 g for strawberry) and number of perforations (10 for plums and 40 for strawberry) for achieving target RH and minimum condensation were selected and validated experimentally with two replicate packages for each fruit type. The actual weight of fruits in each package was 400.4 ± 0.3 g and 458.4 ± 0.2 g for strawberry and plum respectively, which is shown in Fig. 1.

Each package was equipped with an air humidity sensor (Ahlborn, Holzkirchen, Germany) for measurement of temperature and RH. It was made sure that there was no direct contact between fruit and air humidity sensor or packaging film. Data was recorded using a data logger (ALMEMO 2490, Ahlborn, Holzkirchen, Germany) for the entire duration of experiment (72 h).

Mean relative percentage deviation (E) as reported by Mathiasb (2008) used to evaluate the mean divergence of the predicted data from the experimental obtained data (Eq. (28)):

$$E\,(\%) = \left[\sum_{n=1}^{n} \frac{|P_{exp} - P_{pr}|}{P_{exp}} \right] \times \frac{100}{N} \tag{28}$$

4. Results and discussion

4.1. Headspace moisture evolution

Fig. 2 shows predicted and measured headspace RH for packaged strawberry and plum with storage under (a) constant and (b) varying temperature profile, respectively. Relative humidity in all packages of strawberry increased rapidly to 100% due to high rate of moisture loss from fruit surface. Also saturation condition was dominant in package of plum fruits, but there were decreases in headspace RH to 87% in each temperature cycle. As mentioned in section 3.2, there were four steps in cyclic ambient temperature for packaged plum which accordingly affected the headspace RH. The sharp rise of temperature in the first step increased the air capacity to hold water vapour and induced a rapid decrease in RH, in a rate which could not be compensated by fruit moisture loss rate. In the second step during the upper limit of temperature cycle, fruit moisture loss gradually compensated part of the last decrease in RH. In the third step, sharp temperature fall together with fruit moisture loss led to rapid increase in RH. Saturation condition was dominant in the fourth step due to decrease in moisture holding capacity of headspace air at lower temperature (Fig. 2b). There was an excellent agreement between predicted and measured headspace RH with an E (%) equal to 0.006 for strawberries and 0.94 for plums MAHP, showing robustness of simulation program that includes all possible parameters affecting the headspace RH. The experimental results are in agreement with previously published data (Linke and Geyer, 2013; Lu et al., 2013; Song et al., 2002).

The simulation results on cumulative amount of condensation and distribution of condensation on fruit surface and tray wall for packaged strawberry and plum is shown in Fig. 3a and b respectively. Retention time is an index indicating the period in which

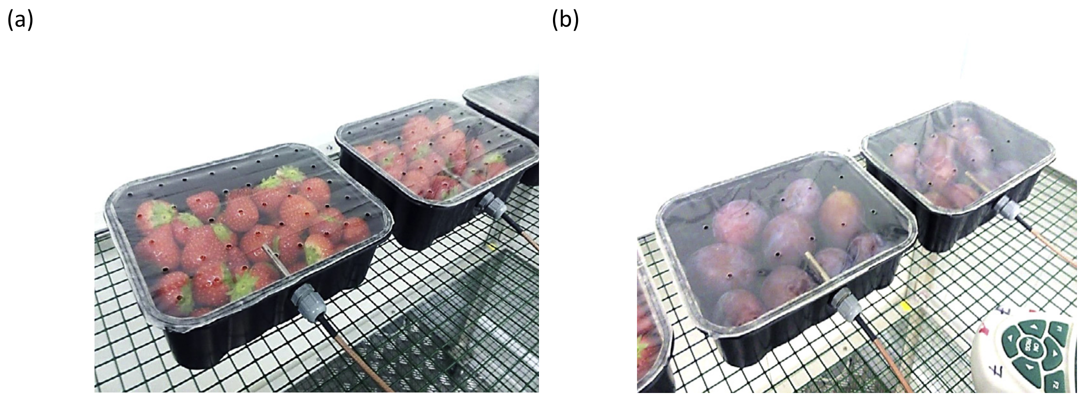

Fig. 1. Modified humidity packaging of (a) strawberry and (b) plum with 40 and 10 macro-perforations, respectively. Storage conditions: 15 °C and 50% ambient humidity.

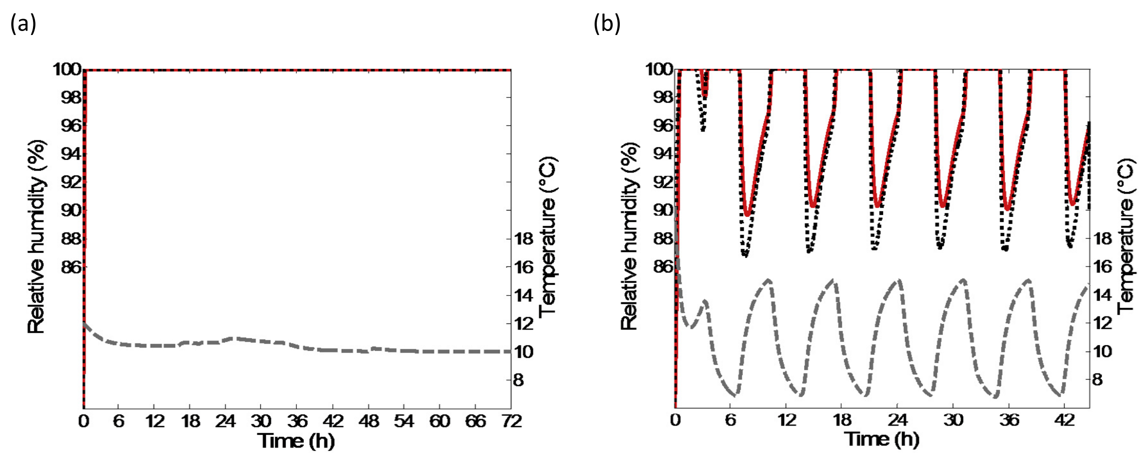

Fig. 2. Predicted (—) and measured (···) headspace relative humidity for storage of packaged (a) strawberry under constant and (b) plum under varying temperature profile (– –).

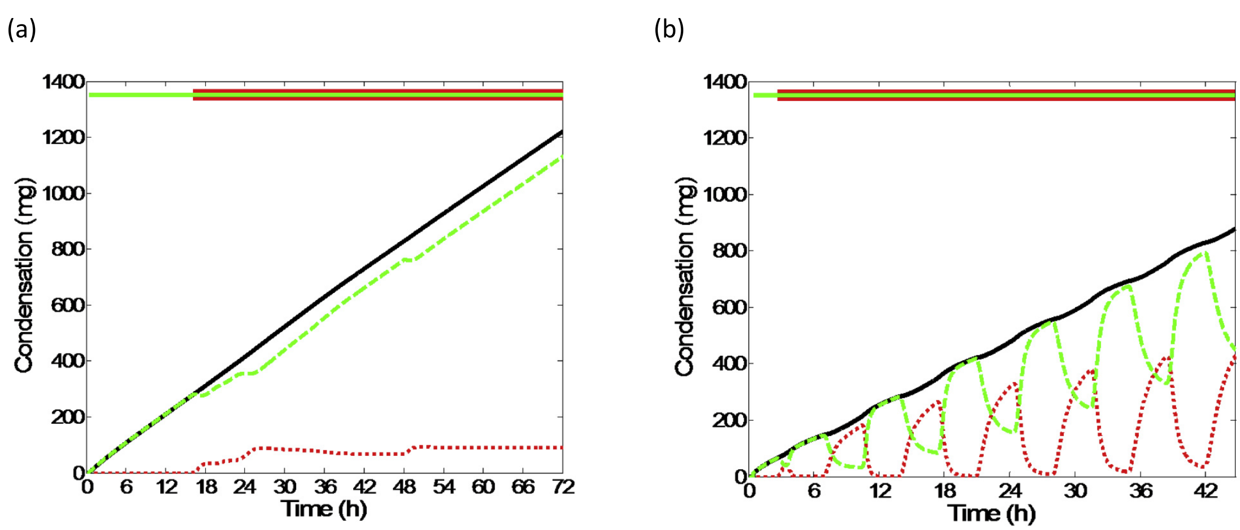

Fig. 3. Predicted condensation dynamics on fruit surface and tray wall for packaged (a) strawberries and (b) plums (total condensation: —), fruit surface condensation: ···, tray wall condensation: – –, retention time on fruit surface (▬), retention time on tray wall (▬).

there exist water vapour condensate on each relevant surfaces regardless its amount. Condensation in both packages started shortly after closing the package lid due to humidity saturation of headspace. Predictions from simulation program showed that condensed water vapour migrated between different surfaces due to temperature fluctuations (Fig. 3). At heating courses in temperature cycle, the condensed water evaporated from tray wall and condensed on fruit surface. The inverse process occurred during cooling courses in temperature cycle. In case of strawberry packages with perforation, ambient temperature was constant, condensation occurred more on tray wall rather than fruit surface. While for plums in which temperature was not constant, the exchange of moisture between fruit surface and tray wall was quite visible. For example, at the beginning of condensation, total condensation was equal to tray wall condensation, and fruit surface condensation was zero, while after 8 h, at the end of first heating course, the position was changed, fruit surface condensation increased to maximum and tray wall condensation decreased to zero. Overall in both cases, cumulative amount of condensation on fruit surface was less than tray wall, as fruit surface had relatively higher average temperature than tray wall due to heat of respiration. Similar result was obtained by Linke and Geyer (2013).

After 72 h storage, the measured total weight loss of packaged strawberry was 1091 mg which was in agreement with the predicted value of 1456 mg. The total moisture loss was predicted 1313 mg, equaling the sum of predicted total condensation (1226 mg) and permeation through the packaging film (82 mg) with a slight difference (5 mg) due to net moisture added to headspace air. The least amount of water vapour permeated was due to relatively high ambient RH (90%) and low water vapour permeability of lidding film.

4.2. Package temperature evolution

Fig. 4 shows predicted and measured temperature evolution of fruit surface, headspace and tray wall of a package containing plums in first 24 h of time. Here the E (%) was 1.95 and 3.18 for headspace and fruit surface temperature in MAHP of strawberry with one perforation. The values of E (%) for headspace, fruit surface and tray wall were 6.51, 8.22 and 8.39, respectively in packaged plums. There was a very good agreement between measured and predicted transient temperatures of packaging component, as E values were lower than 10% indicating a good fit for practical purposes (Van den Berg and Bruin, 1981). Many observations can be made from Fig. 4d. Fruit surface was less affected by ambient temperature followed by package headspace and tray wall surface. This was due to the damping effect of each component when it absorbs part of heat. As the entire package was saturated with humidity, the dew point temperature was equal to headspace temperature.

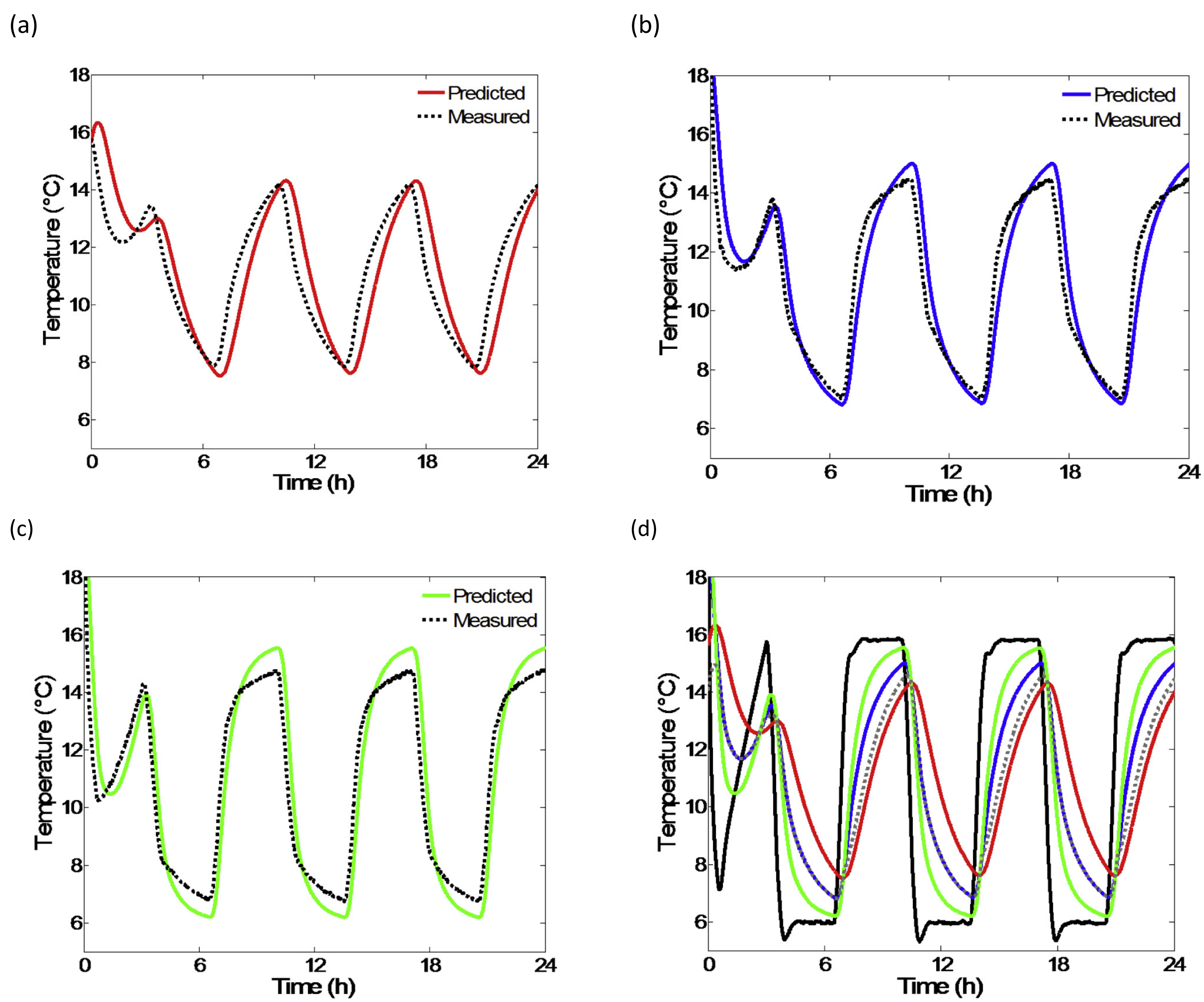

Fig. 4. Measured and predicted temperatures evolution of (a) fruit surface, (b) headspace and (c) tray wall respectively and (d) predicted temperature of all components (fruit surface: ▬, headspace: ▬, tray wall: ▬, dew point: ···), against measured ambient air temperature (▬) for packaged plum.

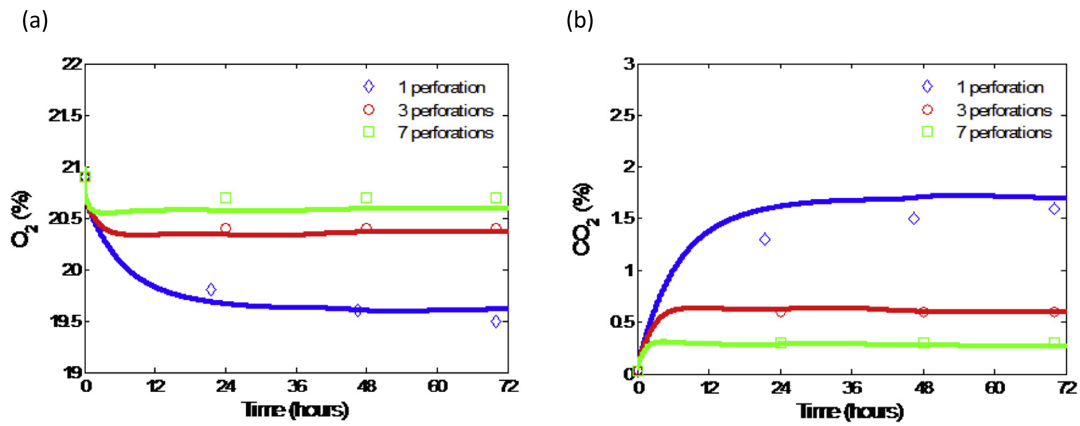

Fig. 5. Headspace gas composition (a) O_2 and (b) CO_2 of packaged strawberry with 1, 3 and 7 perforations (respectively blue, red and green). Symbols are experimental and lines are predicted values. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

4.3. Headspace O_2 and CO_2 evolution

Fig. 5 depicts the effect of the number of perforations on O_2 and CO_2 concentrations in the headspace of packaged strawberry. The number of perforations had an impact on the equilibrium O_2 and CO_2, e.g. with 1 perforation the O_2 was 19.5% whereas with 7 perforations it was only slight modified to 20.7%. Similar findings were reported by Techavises and Hikida (2008) and Sousa-Gallagher et al. (2013). The modified atmosphere (O_2/CO_2) of 19.7/1.3, 20.4/0.6, 20.6/0.3 was achieved after 24 h for packages with 1, 3 and 7 macro-perforations of size 3 mm diameter, respectively. Experimentally measured O_2 and CO_2 concentrations were in agreement with predicted values. It is true that none of macro-perforations resulted into optimum gas atmosphere recommended for strawberry. Optimization of the number of micro-perforations, with much smaller diameter, for achieving optimum modified atmosphere for strawberry was performed. However, it led to saturation humidity and condensation due to insufficient water vapour permeability of the packaging film. On the contrary, achieving modified humidity was feasible by compromising the gas atmosphere. The results presented in this study proved the ability of the simulation program to predict package atmosphere as well as humidity. Finding alternative solutions to achieve both modified atmosphere and humidity is the subject of future studies.

4.4. Further application of simulation program

Table 2 summarizes the data generated by simulation program for both packaging of strawberry and plum. Increasing the temperature increased CO_2 and decreased O_2 equilibrium level in the package headspace for plums and strawberries. Also, the more number of perforations in packaging film led to higher equilibrium level of O_2 and lower equilibrium level of CO_2 which is in agreement with widely published literature (Mahajan et al., 2007; Sousa-Gallagher and Mahajan, 2013; Tano et al., 2007; Techavises and Hikida, 2008). RH inside package was 100% in most combinations of temperature and perforation number. Increasing the number of perforations increased the amount of water vapour permeated out of the package, as seen from the difference in moisture loss and amount of condensation (Table 2). It was in agreement with Fishman et al. (1996) and Rodov et al. (2010) who reported that when the amount of permeation exceeds the amount of moisture loss from fruits, RH will decrease from saturation.

In all combinations of temperature and perforation number, total moisture loss increased with increasing the temperature which is in agreement with previous reports (Mahajan et al., 2008; Sousa-Gallagher et al., 2013). When equilibrium RH was 100%, total moisture loss was constant regardless the number of perforations, while significant decrease, positively dependent on the number of perforations, was observed when RH decreased below saturation level. Condensation occurred when headspace RH was equal to 100%. Total condensation amount increased with increasing the temperature and accordingly higher moisture loss. Increasing the number of perforations decreased the amount of condensation (Table 2). This is due to the fact that more water vapour permeated through the packaging film when perforation number increased which is in agreement with Techavises and Hikida (2008). From the simulated data, it can be seen that equilibrium RH was below saturation level using 40 and 10 macro-perforations for strawberry and plum respectively irrespective of temperature and initial fruit weight. Experimental validation with 40 and 10 macro-perforations on packaged strawberry and plum respectively resulted in no condensation. However, the gas composition in both packaged fruits did not change significantly (20.2% O_2 and 0.28% CO_2) and stayed was close to the air. This was due to bigger perforation diameter used.

The predicted equilibrium headspace RH was 94.0% and 98.8% for strawberries and plums respectively which were very close to measured values of 93.5 and 94.1%, respectively. It is also possible to reduce the number of perforations by using bigger perforation diameter, as the apparent permeability of the film is proportional to the total area of macro-perforations (Techavises and Hikida, 2008). Similarly, the simulation program can be used to design size and number of perforations to achieve equilibrium modified atmosphere alone or in combination with packaging material having higher water transmission rate for water vapour, thus achieving both modified atmosphere and humidity packaging. Further, there is still a scope to improve the capability of simulation program by adding active humidity regulator. This can be done by incorporating the mathematical model for moisture absorption kinetics of such active material.

5. Conclusions

Proper design of modified atmosphere and humidity packaging of fresh fruits and vegetables has been the aim of many researchers especially within the recent years. However, there was always a need to consider various designing aspects and their interactions as well as extending the results to varying environmental conditions affecting whole design problem. The proposed mathematical model

Table 2
Predicted results for O_2, CO_2 and RH at equilibrium, moisture loss and condensation in packaged strawberries and plums under different storage temperatures and packaging conditions (number of perforations and weight of product).

Weight of product (g)		Number of perforations	O_2 (%)			CO_2 (%)			RH (%)			Weight loss (g/g %)			Condensation (g/g %)		
			5 °C	10 °C	15 °C	5 °C	10 °C	15 °C	5 °C	10 °C	15 °C	5 °C	10 °C	15 °C	5 °C	10 °C	15 °C
Strawberry	400	10	20.71	20.43	19.93	0.18	0.30	0.50	100	100	100	0.39	0.70	1.24	0.18	0.40	0.80
		20	20.92	20.79	20.57	0.10	0.16	0.27	99.31	100	100	0.39	0.70	1.24	0	0.16	0.47
		30	20.95	20.90	20.78	0.08	0.12	0.19	88.35	95.27	100	0.45	0.73	1.23	0	0	0.15
		40	20.96	20.93	20.87	0.07	0.10	0.15	81.36	86.99	93.96	0.49	0.79	1.27	0	0	0
	450	10	20.66	20.34	19.78	0.20	0.33	0.56	100	100	100	0.39	0.70	1.24	0.20	0.42	0.83
		20	20.89	20.75	20.49	0.11	0.18	0.30	100	100	100	0.39	0.70	1.24	0.05	0.21	0.54
		30	20.94	20.89	20.73	0.09	0.13	0.21	91.43	98.92	100	0.43	0.70	1.16	0	0	0.26
		40	20.95	20.92	20.85	0.07	0.11	0.16	84.13	90.27	98.09	0.47	0.76	1.23	0	0	0
	500	10	20.61	20.25	19.62	0.22	0.36	0.61	100	100	100	0.39	0.70	1.25	0.21	0.44	0.86
		20	20.86	20.70	20.40	0.12	0.20	0.33	100	100	100	0.39	0.70	1.24	0.08	0.25	0.60
		30	20.93	20.85	20.67	0.09	0.14	0.23	94.26	100	100	0.42	0.69	1.23	0	0.07	0.34
		40	20.95	20.91	20.81	0.08	0.11	0.18	86.72	93.34	100	0.46	0.74	1.22	0	0	0.09
Plum	400	1	19.68	18.77	17.88	0.51	0.82	1.14	100	100	100	0.13	0.22	0.31	0.10	0.17	0.25
		4	20.74	20.53	20.32	0.15	0.24	0.33	100	100	100	0.13	0.22	0.31	0.05	0.10	0.15
		7	20.90	20.80	20.71	0.10	0.15	0.20	96.90	100	100	0.13	0.22	0.31	0	0.03	0.06
		10	20.93	20.88	20.83	0.08	0.11	0.15	82.53	90.58	92.52	0.13	0.22	0.31	0	0	0
	450	1	19.50	18.49	17.51	0.56	0.92	1.26	100	100	100	0.13	0.22	0.31	0.10	0.18	0.25
		4	20.70	20.45	20.21	0.17	0.26	0.36	100	100	100	0.13	0.22	0.31	0.06	0.11	0.16
		7	20.88	20.75	20.64	0.11	0.16	0.22	100	100	100	0.13	0.22	0.31	0.01	0.05	0.08
		10	20.92	20.87	20.81	0.09	0.12	0.16	86.71	95.77	97.93	0.13	0.22	0.31	0	0	0
	500	1	19.33	18.21	17.14	0.62	1.01	1.39	100	100	100	0.13	0.22	0.31	0.10	0.18	0.25
		4	20.65	20.37	20.10	0.18	0.29	0.40	100	100	100	0.13	0.22	0.31	0.06	0.12	0.18
		7	20.85	20.71	20.58	0.12	0.18	0.24	100	100	100	0.13	0.22	0.31	0.02	0.07	0.10
		10	20.92	20.85	20.77	0.09	0.13	0.18	90.91	100	100	0.13	0.22	0.31	0	0.01	0.02

is a comprehensive simulation program, for predicting the dependent variables of packaging design such as gas composition, humidity and water vapour condensation dynamics under varying environmental conditions resembling supply chain of fresh fruits and vegetables based on specific properties of fresh produce and packaging materials. In overall, there was good agreement between measured data from validation experiments performed and predicted data from simulation program supporting previously published works. It was an integrative approach to gain the maximum benefit from previously published literature thus, providing a comprehensive database related to physiological behavior of fresh products under varying environmental conditions and engineering properties of packaging materials. The simulation program can easily replace the costly and time consuming experimental procedures for packaging design for fresh produce.

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Nomenclature

$\boldsymbol{A_1}$ Coefficient (17.625, dimensionless)
$\boldsymbol{B_1}$ Coefficient (243.04 °C)
$\boldsymbol{C_1}$ Coefficient (610.94 Pa)
$\boldsymbol{A}$ Film area (m^2)
$\boldsymbol{A_{p1}}$ Top surface area of package (m^2)
$\boldsymbol{A_{p2}}$ Bottom surface area of package (m^2)
$\boldsymbol{A_{p3}}$ Side surface area of package (m^2)
$\boldsymbol{A_p}$ Total surface area of package (m^2)
$\boldsymbol{A_s}$ Total surface area of product (m^2)
$\boldsymbol{C_a}$ Humid heat of air (J $kg^{-1}K^{-1}$)
$\boldsymbol{C_p}$ Specific heat of fruit
$\boldsymbol{CO_2^{in}}$ Headspace CO_2 concentration (v/v %)
$\boldsymbol{CO_2^{out}}$ Ambient CO_2 concentration (v/v %)
$\boldsymbol{D_1}$ length of top in package assumed as horizontal plate (m)
$\boldsymbol{D_2}$ length of bottom in package assumed as horizontal plate (m)
$\boldsymbol{D_3}$ length of side in package assumed as vertical plate (height of package) (m)
$\frac{dM_{rr}}{dt}$ Rate of moisture loss due to fruit respiration (mg h^{-1})
$\frac{dM_i}{dt}$ Rate of mass change of gas i (i: O_2, CO_2 or H_2O) in headspace (mg h^{-1})
$\frac{dP_i}{dt}$ Permeation rate of gas i (i: O_2, CO_2 or H_2O) through packaging film (mg h^{-1})
$\boldsymbol{e}$ Thickness of polymeric film (m)
$\boldsymbol{E_{aO_2}}$ Activation energy for O_2 respiration
$\boldsymbol{E_{aCO_2(f)}}$ Activation energy for CO_2 respiration
$\boldsymbol{H_{in}}$ Humidity mixing ratio of headspace air (g H_2O/kg air)
$\boldsymbol{h_p}$ Convective heat transfer coefficient between tray wall and air (J $m^{-2}h^{-1}K^{-1}$)
$\boldsymbol{h_s}$ Convective heat transfer coefficient between fruit surface and air (J $m^{-2}h^{-1}K^{-1}$)
$\boldsymbol{H_v}$ Latent heat of vaporization for water (J mg^{-1})
$\boldsymbol{K_{mO_2}}$ Michaelis-Menten constant
$K_{mCO_2(f)}$ Michaelis-Menten constant
$\boldsymbol{K_i}$ Permeability coefficient of film to gas i (i: O_2, CO_2 or H_2O) (mg $m^{-2}h^{-1}Pa^{-1}$)
M_{cond} Total amount of water vapour condensate inside package(mg)
MH_2O_{air} Total amount of water inside the package (mg)
MH_2O_{max} Maximum amount of water vapour in headspace air (mg)
N_p Number of perforations of film
O_2^{in} Headspace O_2 concentration (v/v %)
O_2^{out} Ambient O_2 concentration (v/v %)
P_{atm} Atmosphere pressure (Pa)
P_{eff} Effective permeability of macro-perforations (mg $h^{-1}m^{-2}Pa^{-1}$)
P_{in} Headspace partial pressure of water vapour (Pa)
P_{out} Ambient partial pressure of water vapour (Pa)

P_{sat}	Partial pressure of water vapour at saturation (Pa)
RH_{in}	Package internal relative humidity (%)
RH_{out}	Ambient relative humidity (%)
R_{O_2}	O_2 consumption rate of fruit (mg $kg^{-1}h^{-1}$)
R_{CO_2}	CO_2 production rate of fruit (mg $kg^{-1}h^{-1}$)
RQ_{OX}	Respiratory quotient (0.91)
R_p	Radius of the perforations (mm)
T	Temperature (°C)
T_i	Package headspace temperature (°C)
T_o	Ambient temperature (°C)
T_s	Fruit surface temperature (°C)
T_t	Tray wall surface temperature (°C)
T_{ref}	Reference temperature (10 °C)
V_f	Package headspace volume (m^3)
V_p	Total volume of fruits (m^3)
V_t	Package total volume (m^3)
$Vm_{O_2}^{ref}$	Maximum O_2 consumption rate at reference temperature (mg $kg^{-1}h^{-1}$)
$Vm_{CO_2(f)}^{ref}$	Maximum CO_2 production rate at reference temperature (mg $kg^{-1}h^{-1}$)
W_p	Weight of fruit (kg)
W_a	Mass of headspace dry air (kg)
λ	
ρ_{air}	Density of air (kg m^{-3})
ρ_{wv}	Density of water vapour (kg m^{-3})

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