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Stochastic modelling for virtual engineering of controlled atmosphere storage of fruit

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ABSTRACT

Long term storage of pear fruit requires low temperature and conventionally uses controlled atmosphere (CA) conditions to reduce respiration and consequent quality loss. Sub-optimal storage conditions may lead to physiological disorders and loss of product. Stochastic variability of the properties of fruit introduces uncertainty in storage design and operations and could result in severe quality loss. Taking such variability into account in simulation models for virtual engineering will allow to assess the uncertainty of the process and determine confidence limits for the operation. Gas exchange in pear fruit during controlled atmosphere storage was studied using a continuum diffusion–respiration model, taking into account stochastic variation of the 3D morphology, the diffusivity of oxygen and carbon dioxide and the maximal respiration rate. Different geometries were generated using a statistical shape generation algorithm for 3D morphology, that was automatically incorporated into the gas exchange model. Similarly, tissue diffusivity was computed using a 3D tissue microstructure database. Simulation results showed that internal O_2 and CO_2 gas profiles in fruit were highly affected by variation of diffusivities, maximal respiration rate and the 3D morphology of fruit. The model was further used to evaluate incidence to fermentation at different reduced O_2 levels of storage condition. The risk of fermentation inside the fruit predicted by the gas exchange model rapidly increased in response to decreasing external O_2 levels. The virtual simulation tool confirms that picking time and fruit size are important criteria for proper control of CA storage. While applied here to pear fruit, it can easily be extended to other commodities.

1. Introduction

Pome fruit are an important fresh food product consumed worldwide. After harvest, fruit are often stored under controlled atmosphere (CA) conditions with reduced O_2 and increased CO_2 levels in combination with a low temperature to extend their commercial storage life. In such conditions, gas exchange inside the fruit affects the respiration process. Bad engineering and control of the storage rooms may result in sub-optimal storage conditions that may lead to physiological disorders and loss of product. In 'Conference' pears (Pyrus communis L.), the physiological disorder is characterised by softening and browning of tissue near the core and is associated with the development of cavities (Franck et al., 2007; Veltman et al., 2003a, 1999) that cause economic losses (Lammertyn et al., 2000; Veltman et al., 2003a; Zerbini and Rizzolo, 2002). The main hypothesis for explaining the occurrence of browning is that hypoxia inside the fruit might occur, followed by a switch from respiration to fermentation. The low energy yield of the latter is insufficient for repairing membrane damage, and cell death may result (Herremans et al., 2013a,b; Ho et al., 2011; Lammertyn et al., 2000; Pedreschi et al., 2009; Peppelenbos and Oosterhaven, 1998; Saquet et al., 2003; Streif et al., 2003; Veltman et al., 2003b; Zhou et al., 2014). The development of disorders during postharvest ripening and storage of fruit also depends on a range of preharvest factors such as climate conditions. Other factors that have been considered to be influencing the development of the disorder are the size/weight of the fruit and the picking date (Ho et al., 2010a; Lammertyn et al., 2000; Li et al., 2011). Over-mature (late picked) and large fruit have been shown to be more susceptible to core breakdown during storage (Franck et al., 2007; Lammertyn et al., 2000; Verlinden et al., 2002).

Computer aided engineering through mathematical modelling of the process has been used as a tool for quantification of the fruit quality during storage (Bosch et al., 2013; Fukuda et al., 2014; Ho et al., 2013; Pinheiro et al., 2013). As there are no noninvasive

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measurement techniques available for monitoring respiratory gas concentrations in fruit during CA storage, gas transport models have been used to evaluate gas transport and respiratory gaseous exchange of fruit. We have previously developed models operating at different spatial scales, from the macroscale (Ho et al., 2011, 2008; Lammertyn et al., 2003; Mannapperuma et al., 1991; Verboven et al., 2013) to the microscale level (Ho et al., 2011, 2009; Verboven et al., 2013, 2012) in a multiscale framework and validated them successfully for different apple and pear fruit cultivars (Ho et al., 2010b, 2008). Such modelling has shown that the local gas concentrations and the respiration rate inside fruit differs between cultivars, due to differences in diffusion and respiration properties, shape and size. As a result, optimal storage conditions differ between fruit cultivars (Ho et al., 2013). Because diffusion and respiration properties and fruit shape affect gas exchange in CA storage, variability of these parameters potentially introduces large uncertainty in respiration during storage. Process design should thus account for the effect of variability and predict confidence limits of optimal conditions rather than fixed values (Hertog et al., 2007; Nicolaï et al., 2011; Scheerlinck et al., 2001).

The observed variability of diffusion and respiration properties of fruit is large (Ho et al., 2011, 2010b). The shape of biological products is often complex, and rather difficult to acquire and describe (Goñi et al., 2008; Mebatsion et al., 2011). In addition, a large variability is found between species and cultivars. We have, however, been able to generate 3D computer models of pome fruit (Rogge et al., 2013). The resulting geometrical models have the same variability as the biological variability in the original biological products. While these 3D geometrical models are directly available as CAD models, numerical modelling of respiratory gas transport phenomena inside the fruit taking into account 3D geometrical variation of biological products has not been achieved yet.

The objective of this contribution was to model the gas exchange in pear fruit taking the effects of biological variability into account. First, the variability distribution of relevant model parameters is determined, including shape, tissue structure and respiration rate. Then, stochastic simulations are used to evaluate the uncertainty of internal respiratory gas concentrations of the fruit and evaluate the consequences for susceptibility to storage disorders under optimal and sub-optimal conditions.

2. Material and methods

2.1. Materials

Pears (Pyrus communis 'Conference') were picked from the experimental orchard of the Research Station of Fruit Growing (Velm, Belgium). Fruit was harvested at two stages: in the optimal picking period (on 9th September, 2010) and in the late picking period (on 16th September, 2010). Fruits were cooled and stored according to commercial protocols for a period of 21 days at −1 °C followed by controlled atmosphere conditioning (2.5 kPa O_2, 0.7 kPa CO_2, −1 °C) up to the time of the experiment. Picking dates and cooling procedures were according to optimal commercial practices used for long-term storage of fruit.

2.2. 3D shape generation

An enhanced version of the geometric model generator described in Rogge et al. (2015) was used to create the required 3D geometric models of pear fruit. The model generator is able to accurately represent all shape features of the 3D outer contour of the pears. The model generating algorithm that uses a 2D Fourier series expansion was developed based on surface contours extracted form X-ray Computed Tomography images of 66 'Conference' pears (Rogge et al., 2013). After statistical analysis of the obtained descriptors for all pears, new descriptors were generated, representing the studied distributions of descriptors. With the inverse of the shape description method, these new descriptors were transformed into smooth geometries, fit as CAD import for the simulations. The geometries were meshed with Comsol 3.5 (Comsol AB, Stockholm).

2.3. Diffusion–reaction model of gas exchange in pear fruit

The diffusion–reaction model of gas exchange that we developed earlier (Ho et al., 2010b, 2008) was used for stochastic simulations in this work. In this approach, tissues are considered to be homogeneous continuum materials. The effect of microstructural features (porosity and tortuosity) on gas transport is incorporated in the apparent value of the tissue properties.

Gas concentration gradients are the driving force for gas exchange. The continuum model thus contains diffusion and reaction terms:

$$\alpha_i \frac{\partial C_i}{\partial t} = \nabla \cdot D_i \nabla C_i + R_i \tag{1}$$

with α_i the gas capacity of the component i (O_2 and CO_2) of the tissue (Ho et al., 2010b), D_i ($m^2\ s^{-1}$) the apparent diffusion coefficient of the tissue, R_i ($mol\ m^{-3}\ s^{-1}$) the reaction term of the gas component i related to O_2 consumption or CO_2 production, (m^{-1}) the gradient operator, and t (s) the time. The time derivative in the left side of Eq. (1) represents the concentration changes over time t (s) and becomes zero at equilibrium. Based on preliminary calculations we found that permeation could be neglected.

The gas capacity α_i is defined as:

$$\alpha_i = \varepsilon + (1-\varepsilon) \cdot R \cdot T \cdot H_i = \frac{C_{i,\text{tissue}}}{C_{i,g}} \tag{2}$$

where ε is the porosity of tissue, $C_{i,g}$ ($mol\ m^{-3}$) and $C_{i,\text{tissue}}$ ($mol\ m^{-3}$) are the concentrations of the gas component i in the gas phase and the tissue, respectively. The concentration of the compound in the liquid phase of fruit tissue normally follows Henry's law represented by the constant H_i ($mol\ m^{-3}\ kPa^{-1}$). R ($8.314\ J\ mol^{-1}\ K^{-1}$) is the universal gas constant and T (K) the temperature.

A non-competitive inhibition model Hertog et al. (1998), Ho et al. (2010b), Lammertyn (2001), Peppelenbos and van't Leven (1996) is commonly used to describe consumption of O_2 by respiration:

$$R_{O_2} = -\frac{V_{m,O_2} \cdot C_{O_2}}{(K_{m,O_2} + C_{O_2}) \cdot \left(1 + \frac{C_{CO_2}}{K_{mn,CO_2}}\right)} \tag{3}$$

with V_{m,O_2} ($mol\ m^{-3}\ s^{-1}$) the maximum oxygen consumption rate, C_{O_2} ($mol\ m^{-3}$) the O_2 concentration, C_{CO_2} ($mol\ m^{-3}$) the CO_2 concentration, K_{m,O_2} ($mol\ m^{-3}$) the Michaelis–Menten constant for O_2 consumption, K_{mn,CO_2} ($mol\ m^{-3}$) the Michaelis–Menten constant for non-competitive CO_2 inhibition, and R_{O_2} ($mol\ m^{-3}\ s^{-1}$) the O_2 consumption rate of the sample.

The equation for production rate of CO_2 consists of an oxidative respiration part and a fermentative part (Peppelenbos and van't Leven, 1996):

$$R_{CO_2} = -r_{q,ox} \cdot R_{O_2} + \frac{V_{m,f,CO_2}}{\left(1 + \frac{C_{O_2}}{K_{m,f,O_2}}\right)} \tag{4}$$

with V_{m,f,CO_2} ($mol\ m^{-3}\ s^{-1}$) the maximum fermentative CO_2 production rate, K_{m,f,O_2} ($mol\ m^{-3}$) the Michaelis–Menten constant of O_2 inhibition on fermentative CO_2 production, $r_{q,ox}$ the respiration quotient at high O_2 concentration, and R_{CO_2} ($mol\ m^{-3}\ s^{-1}$) the CO_2

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